



University of the  
West of England

# Model Based Engine Efficiency

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## **Abstract**

Internal Combustion Engines have become more refined since their first appearance in automotive applications. A modern engine has sensors, actuators and controllers added to the standard internal combustion engine in order to achieve higher levels of fuel economy and lower emissions while still retaining a desirable level of performance.

Much of the details of combustion are still not well understood, prompting fundamental investigation. Furthermore, to further perfect internal combustion engines and implement future technologies, a deep understanding of the underlying principles is required, in order to intelligently specify the requirements of said future technologies.

Currently two main branches of internal combustion engines exist, that of the spark ignition, and that of compression ignition engines. The latter has not been as common in road vehicles until recent years. This increase is particularly pronounced in European markets.

Without any clear indication of which is the definite way forward until Zero Emission Vehicle (ZEV) are a reality, one must consider both. It seems that compression ignition engines are not as well documented as spark ignition engines. This was also apparent from the lack of equal understanding by professionals in the industry. So much so, that in general, very few authorities of the internal combustion engine exist. The best known in the field is Heywood, John B.

The author therefore proposed to develop a set of tools to model internal combustion engines including the often omitted compression ignition engines. This would provide a foundation for further investigation of other current and future technologies such as variable valve timing.

The author has a particular interest in compression ignition engines since this is the area in which the author has the least experience. The author's industrial experience at DENSO UK Sales Ltd., in preparation for the author's work in DENSO AUTOMOTIVE Deutschland GmbH's European research and development centre at the Aachen Engineering Centre and DENSO Japan, this provided the ideal setting to make this work a beneficial investment.

The aims of this investigation, in a simpler sense, were to understand a wide number of topics related to combustion. Apply this knowledge in a useful manner for the author and others in the future, who might require to understand internal combustion engine from a scientific perspective. This was set to be in the form of a simulation package.

Together with discussions and collaboration with academics from the University of the West of England and colleague Mark Elliot, a set of modular tools have been developed (referred to as Engine Sim) that show desirable levels of correlation with test data acquired from the University, publications of previous authors and third party acquired test data.

Perhaps the most surprising outcome to the author has been the remarkable similarity between modern compression ignition and spark ignition engines, and their similarity in modelling approach.

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## Nomenclature

$c_p$	Specific heat at constant pressure
$c_v$	Specific heat at constant volume
$c_{p,f}$	Specific heat at constant pressure of frozen mixture
$c_{p,r}$	Specific heat at constant pressure of reaction
$CN$	Cetane Number
$E$	Error / Energy imbalance
$h_f$	Specific enthalpy
$m_c$	Mass of charge
$m_f$	Mass of fuel
$\eta_c$	Combustion efficiency
$p$	Pressure
$\eta_{TH}$	Thermal efficiency
$q$	Specific heat transfer
$q_a$	Specific heat added
$q_n$	Net specific heat transfer
$q_r$	Specific heat rejected
$Q$	Heat transfer
$r$	Compression ratio
$r_c$	Cut-off ratio
$r_e$	Expansion ratio
$R$	Gas constant
$u$	Specific internal energy
$U$	Internal energy
$t$	Time
$t_{id}$	Ignition delay period
$T$	Temperature
$v_p$	Average piston speed
$V$	Instantaneous chamber volume
$V_c$	Compressed volume
$V_s$	Swept volume
$x_b$	(Mass) fraction burn
$\gamma$	Isentropic index
$\theta$	Angular position
$\phi$	Equivalence ratio

## **Abbreviations**

<b>A/F</b>	Air to fuel ratio
<b>ATDC</b>	After Top Dead Centre
<b>BDC</b>	Bottom Dead centre
<b>BTDC</b>	Before Top Dead Centre
<b>CI</b>	Compression Ignition
<b>IC</b>	Internal Combustion
<b>SI</b>	Spark Ignition
<b>TDC</b>	Top Dead Centre
<b>CA</b>	Crank Angle

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## **1. Introduction to the Internal Combustion Engine**

Internal combustion (IC) engines which had any real commercial success originated in the 1860s. Such engines had a maximum power of 6 horsepower and efficiency no greater than 5%. (Cummins, Jr., C. L., 1976)

The designs that followed were those of Nicolaus A. Otto (1832-1891) and Eugen Langen (1833-1895). Their engines produced roughly the same power however with a thermal efficiency of 11%. (Heywood, John B., 1988)

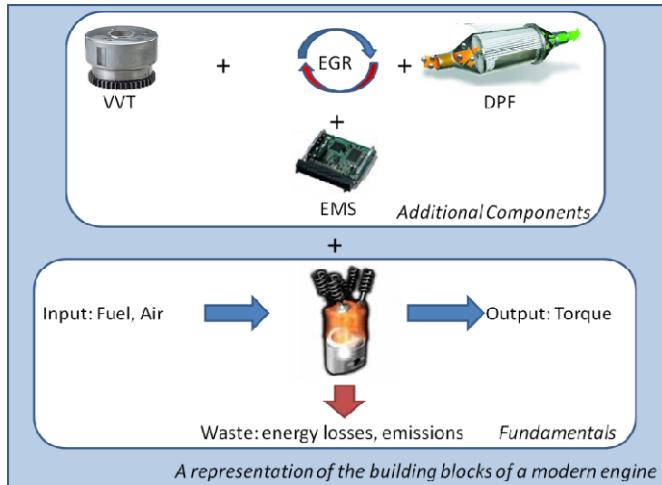
The work of French physicist Said Carnot and French railway engineer Beau de Rochas were the first to define the basic four stroke concept. Though these contributions were not given much notice at the time, their inclusion of a compression stroke would prove vital to virtually any commercial IC engine to date. (Milton Brian E., 1995)

Otto would produce the first engine prototype (known as the Otto ‘Silent’ engine) in 1876 which included the compression stroke (at a compression ratio of 2.5:1). Otto had not properly understood the reason for the success of this engine. Otto believed the increase in efficiency of this engine to about 14% was due to the stratification of the charge, however Dugald Clerk who was the first to perform thermodynamic analysis of the Otto cycle, demonstrated otherwise. It was the compression stroke which gave a greater expansion ratio, thus raising the efficiency. Nonetheless, most credit Otto as the father of the modern IC engine as this design sold about 50,000 units. (Heywood, John B., 1988 and Stone, Richard, 1999)

The original Otto engine was slow rotating and low power. The engine design went through several refinements by engineers such as Gottlieb Daimler, Karl Benz, Wehelm Maybach and Rober Bosch. These engineers raised the engine speeds, introduced acceptable power-to-weight ratios and invented better ignition systems by the late 1890s. The final major contribution was probably that of the compression ignition engine by Rudolf Diesel. Rudolf Diesel was the first inventor to show clear scientific approach to engine design as opposed to just refinement through practical experience. (Milton Brian E., 1995)

The IC engine has come a long way from its original practical forms, however most authorities such as Heywood, John B. (1988) and Milton Brian E. (1995) as well as Ricardo, Harry R. and Hempson, J.G.G. (1968) tend to agree with the author’s personal opinion that modern commercial road engines (aside from other designs such as the Wankel Rotary engine which came much later in 1957 and are used in a limited range of vehicles today) are very similar in principle to that proposed and built by Otto and the changes are that of refinements.

Such modern requirements have raised power outputs considerably as well as the raised efficiency of the IC engine. Most of the additions found on modern state of the art engines, with additional components such as intelligent stop-start (ISS), variable valve timing (VVT), diesel particulate filters (DPF), exhaust gas recirculation (EGR) and advanced control engine management systems (EMS), may be regarded as complex ‘bolt on’ devices designed to improve engine efficiency, bringing it closer to the theoretical value or to comply with stricter demands of emission control.



**Figure 1 - Representation of a modern engine**

Even though practically no modern engine is commercially available without such ‘extra’ systems (as depicted in Figure 1), it is impossible to study their influence or importance without properly understanding the fundamentals of IC engines. It is these fundamentals that dictate the purpose or functioning mechanism of these additional devices and systems.

World War I induced progress in understanding the effect of combustion such as that of the problems of knock and possible additives to overcome this. From the early 1900s to date the greatest design factors forcing internal combustion advance has been the need for higher fuel economy and in the more recent decades, the control of urban air pollution. (Heywood, John B., 1988)

One of the earliest devices aimed purely at emission control was the positive crank case ventilation valve (PCV) applied as a mandatory requirement in California as deemed by the California Air Resource Board (CARB) introduced this requirement in 1961 to deal with the deteriorating air quality. British manufacturers had already been utilising this device as it allows un-oxidised or partially oxidised gases leaking past the piston to be return to the combustion chamber having gone through the crankcase. Full emission control legislation followed in several parts of the world, and by the mid-1970s, Japan, Canada and Australia had introduced such controls. (Milton Brian E., 1995)

Hydrocarbon compounds (HC) and carbon monoxide (CO) were the original pollutant concerns, however with the additional consideration of nitrogen-oxygen compounds (NO<sub>x</sub>), a new level of complexity arose. HC and CO compounds required oxidation to be removed, however NO<sub>x</sub> required reduction. This initiated new research programs in the USA with experimental based research and engine modelling investigation. (Milton Brian E., 1995)

The 1971 oil crisis caused a stir, as the common practice for emission control produce engines with higher fuel consumption. This promoted further combustion engine research. Research has since remained on this course of pre-emission control and higher engine efficiency, leading to the CARB emissions standards of Ultralow and Zero emission level vehicles). (Milton Brian E., 1995)

For the author to make any further analysis of current and potential technologies, it was crucial to:

- Develop an understanding of IC engine fundamentals.
- Create a simulation framework to explore and simulate these fundamentals.
- Use the simulation to run “what if” scenarios

## 2. Literature Survey

Common modern IC engines for road vehicles are predominantly divided into two main categories:

- Spark ignition (SI) usually associated with gasoline fuel
- Compression ignition (CI) usually associated with diesel fuel

SI engines are sometimes subdivided into two modes of operations – stratified charge combustion and homogenous charge combustion. Heywood, John B. (1988) and Milton Brian E. (1995) both attribute the origin of the stratified charge concept dating back to the Otto ‘silent’ engine. However, the author is of the opinion that when looking at the current state of technologies, SI stratified combustion is better considered a subset of the generic SI combustion category as stratified combustion is more commonly found as a mode of operation of what is otherwise a regular direct-injection homogenous charge SI engine, for low to medium load control similar to the concept of CI engines.

Throughout this investigation, only **four-stroke** engines were considered and discussed.

### 2.1 SI Engines - Homogenous

SI engines of the homogenous charge combustion type involve four strokes (as shown in Figure 2). The operation goes through the following steps:

- Intake stroke:** Induction of air/fuel charge through the open inlet valves with the exhaust valves closed.
- Compression stroke:** Compression of charge, raising the pressure and temperature of the charge with both valves closed.
- Firing:** Igniting the charge with both valves closed.
- Power stroke:** Expansion of charge with both valves closed.
- Exhaust stroke:** Removal of combustion products through the open exhaust valves with the inlet valves closed.

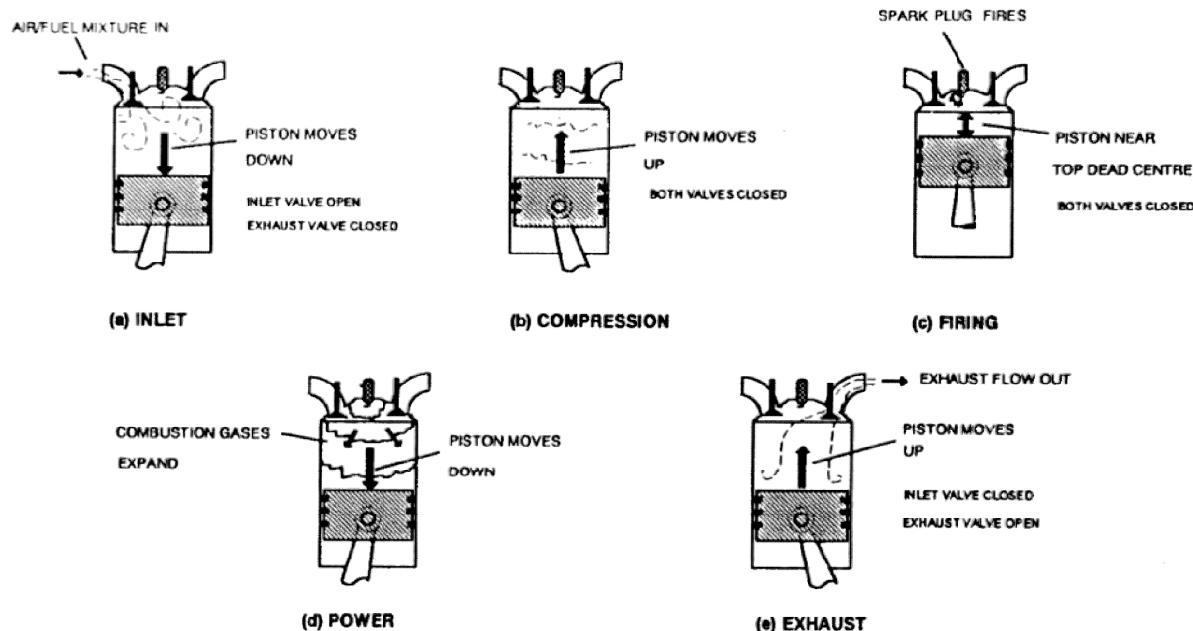


Figure 2 - Spark Ignition Homogenous Strokes (Milton Brian E., 1995)

It is worth noting the important influential parameters on the performance of such a SI engine.

*Compression ratio:* Based on the work of Dougald Clerk and Nikolaus August Otto, it was clear that a higher compression ratio increased the thermodynamic gains and overall efficiency. (Milton Brian E., 1995)

*Fast Burn:* Cycle analysis shows the benefit of faster burn rates. This is achieved by proper head design delivering the correct amount of turbulence and turbulent flame propagation in order to aid a lean mixture to burning rate (lean mixtures burn more slowly than a stoichiometric one). (Milton Brian E., 1995)

*Lean Burn:* A lean burn engine has a higher ratio of specific heats during the cycle which can be shown to be beneficial as long as the desired burn rate may be maintained. This also automatically reduces CO and HC emissions, replacing less fuel efficient emission control strategies. This is limited by misfire and cycle-by-cycle variability which could negate the advantages. (Milton Brian E., 1995)

*Improved control and optimisation of the engine:* Optimising A/F ratios, ignition/injection timing, and exhaust gas recirculation between cylinders for different steady-state and transient speed-loads points all help achieve control over the engine efficiency under the constraints of exhaust emissions. Based on the work experience of the author in engine control, it can be said that most engine control is highly model based (thanks to the more viable price of computing power for an engine control unit) in order to predict parameter optimisation during engine operation for any given feasible running condition (environmental, engine speed-load, etc). (Milton Brian E., 1995)

*Reduce engine size:* For the same maximum power, smaller engines will be operating at a higher mean effective pressure (MEP) making the frictional and pumping losses a smaller proportion of the useful work out. This is particularly beneficial when engine is operating at part throttle. (Milton Brian E., 1995)

Using multiple valves, complex combustion chamber design, turbochargers, and multipoint fuel injection all obviously incur higher investment cost and cost to manufacture (due to the larger quantity of components of higher complexity) which is ultimately paid out by the end customer. (Milton Brian E., 1995)

### 2.2.1 SI Engines - Stratified

This engine design could operate at near optimum compression ratio without risk of auto-ignition (and hence knock). This permits the engine to be controlled by varying the injected fuel quantity (and hence global A/F ratio) as opposed to throttling – similar to that in CI engines. The reduction in throttling helps reduce pumping losses – one of the main benefits of CI engines. The biggest technological barrier has been the development of a high pressure direct injection system and nozzle design, producing sufficient fuel mixing while retaining stratification. (Milton Brian E., 1995)

## 2.3 CI Engines

Compression ignition engines may vary more than SI engines. These are even available with bore diameters as big as 1m operating at speeds of 100rev/min. These are considered beyond the scope of this work as they are not directly relevant to the automotive industry. (Milton Brian E., 1995)

There are two main types of CI engines: a) direct injection (DI) where fuel is sprayed into the combustion chamber and b) indirect injection (IDI) where fuel is sprayed into a pre-chamber producing a fuel rich mixture through high swirl and/or turbulence.

CI engines involve four strokes (as shown in Figure 3). The operation goes through the following steps:

- Intake stroke:** Induction of air through the open inlet valves with the exhaust valves closed.
- Compression stroke:** Compression of air, raising the pressure and temperature of the air with both valves closed.
- Fuel Injection:** Fuel is injected and ignites in the presence of the hot and pressurised air.
- Power stroke:** Expansion of charge with both valves closed.
- Exhaust stroke:** Removal of combustion products through the open exhaust valves with the inlet valves close.

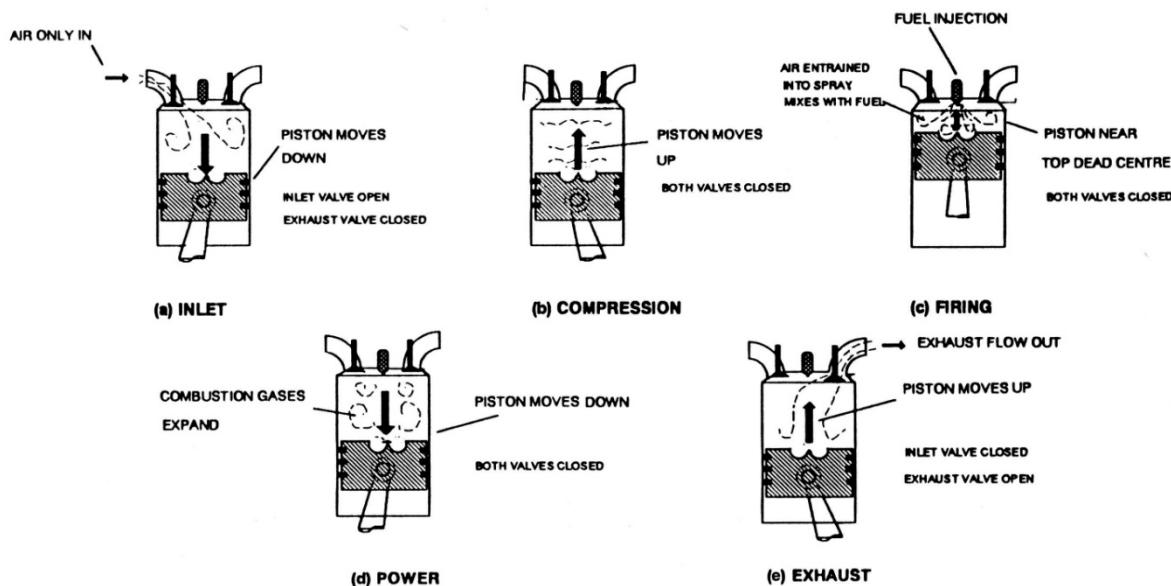


Figure 3 - Compression Ignition Strokes (Milton Brian E., 1995)

IDI CI, partially premixes the fuel as fuel-rich mixture in a pre-chamber and by doing so, generates high swirl and/or turbulence. This mixture undergoes initial combustion within the pre-chamber and is then expelled into the main combustion chamber for its main oxidisation. Such engines are known to be less efficient but have higher speed-load capabilities over DI. CI is limited by the ignition delay of diesel fuel. This is overcome by high pressures and temperatures. turbocharging may be one means of doing so, thus increasing the power-to-weight ratio without reducing the air/fuel ratio. (Milton Brian E., 1995)

This turbocharging trend combined with the further combustion chamber optimisation and injection spray pattern analysis has led to diesel engines becoming more common especially in the European market. (Milton Brian E., 1995)

## 2.3 Current and Future Engine Trends

The years 2000-2006 have seen the advent for engines that can run in homogenous and stratified modes (and blend of the two concepts). However, the recent conferences attended in recent years by the author have shown a very recent decline of investment in stratified research. Immediate engine improvements trends seem to lie in better diesel engines or downsized, cooled exhaust gas recirculation (EGR) and turbocharging, while homogenous charge compression ignition (HCCI) and premixed-controlled compression ignition (PCCI) are seen as possible long term solution. These latter concepts further bring closer CI and SI closer together than they already are which will become more apparent when looking at the thermodynamics of the Otto cycle and Diesel cycle.

## 2.4 Cycle Analysis

Cycle analysis is a fundamental and required step to understanding the key effects, relationships and limitations of various engines. This analysis has permitted engines to reach the complex design state they are in today. Milton Brian E.(1995)

The original tool for this form of analysis was the standard air cycle first developed by Dugald Clerk towards the end of the nineteenth century. Modern day computing has permitted more complex simulations and analysis with finer steps to be run involving more complex thermodynamic cycles (sometimes referred to as zero dimensional) based on the standard air cycle. (Milton Brian E., 1995)

The use of sub models may be applied to include specific phenomena such as burning rates or emission rates. (Milton Brian E., 1995)

The following are standard equations used throughout the analysis of standard air cycles. The equations have been arranged in a form that is most beneficial to the sections ahead and are derived from the thermodynamic laws and cycle analysis published by Heywood, John B. (1988), Milton Brian E. (1995), Turns, Stephen R. (2000), Eastop, T.D. and McConkey, A. (1993) and Rogers and Mayhew (1992).

Lower case  $w$  and  $q$  are used to indicate intensive energies (J/kg) while upper case  $W$  and  $Q$  are used to indicate extensive energies (J).

The first law of thermodynamics for fixed mass of a closed system may be such that positive values are energies entering the system and negative values are energies lost from the system:

$$q - w = \Delta u \quad (1)$$

The work of a complete cycle (ignoring pumping loss) is the net work over a cycle  $w_n$ . The net work may be the sum of the (positive) work done (by the system) during expansion  $w_e$  and the (negative) work done (on the system) during compression  $w_c$ .

$$w_n = w_e + w_c \quad (2)$$

Similarly the net heat flow through the system is denoted as  $q_n$  which is the (positive) heat added (to the system)  $q_a$  together with the (negative) heat rejected (from the system)  $q_r$ .

$$q_n = q_a + q_r \quad (3)$$

For a complete cycle, the system returns to its original state (temperature, volume, internal energy) and thus there is no net change in internal energy. Thus for a cycle, (1) may be written as:

$$w_n = q_n \quad (4)$$

Thermal efficiency is defined as the ratio of net work output to net heat added:

$$\eta_{TH} = \frac{w_n}{q_a} \quad (5)$$

Or as:

$$\eta_{TH} = \frac{q_n}{q_a} \quad (6)$$

Substituting (3) and simplifying defines thermal efficiency as:

$$\eta_{TH} = 1 + \frac{q_r}{q_a} \quad (7)$$

A more useful measure than net work is the indicated mean effective pressure as this value divides the net work output by the displacement volume, making it more useful when comparing different engines of different size.

$$imep = \frac{W_n}{V_s} \quad (8)$$

Compression ratio  $r$  is defined as:

$$r = \frac{\text{swept volume}}{\text{clearance volume}} \quad (9)$$

## 2.4 Geometric Model

A geometric model is necessary to relate crank angle to volume; it would also be used to relate engine speed with the rate of change of volume and/or the change in time. This is particularly important when consider more complex combustion simulation involving reaction rates.

$$V = V_c \left(1 + \frac{1}{2}(r - 1)(R + 1 - \cos \theta - (R^2 - \sin^2 \theta)^{\frac{1}{2}})\right) \quad (10)$$

The relation is straight forward from the engine geometry and easily derived (Heywood, John B., 1988).

All the modelling work will be based on crank angle (CA) as the independent variable, and volumes will be calculated as a function of CA.

### 2.4.1 Otto Cycle

This is regarded as the most useful and representative cycle for SI engines and modern high speed CI engines (as opposed to the standard diesel cycle).

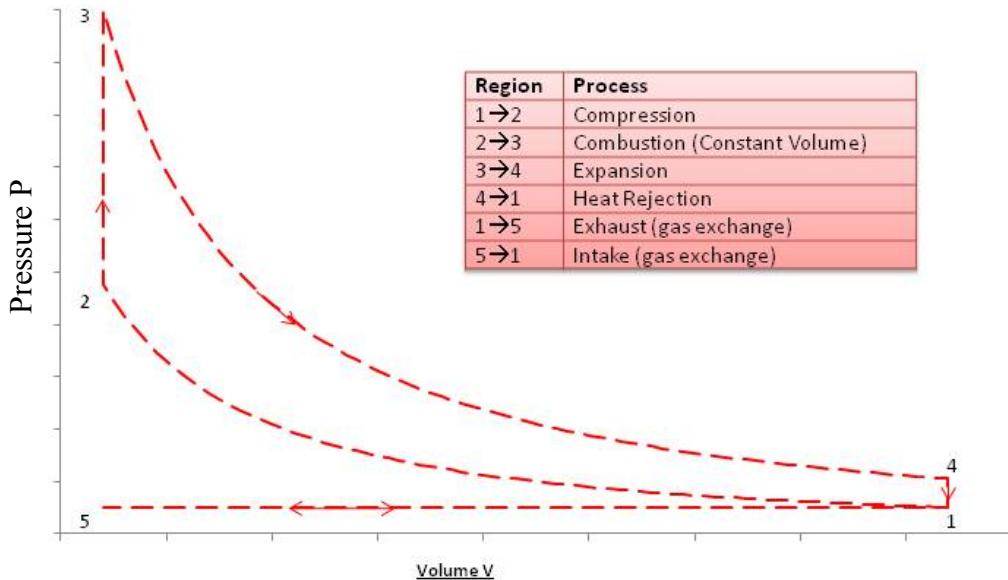


Figure 4 - Air Standard Otto Cycle

Air standard Otto cycle processes (ignoring gas exchange):

- 1 $\rightarrow$ 2 Isentropic compression from the initial condition (air in the cylinder at the end of the intake)
- 2 $\rightarrow$ 3 Constant volume heat addition
- 3 $\rightarrow$ 4 Isentropic expansion of the heated gas to produce work
- 4 $\rightarrow$ 1 Constant volume heat rejection to atmosphere

1. Isentropic compression is a reasonable approximation in spite of the carried-over turbulence through the intake and that of the compression process itself, since the temperature range of the compressed fluid is likely to range only between 40°C to 400°C with a cylinder wall in excess of 100°C. Therefore the net heat transfer is likely to be relatively small. (Milton Brian E., 1995)

2. The heat addition is likely to be the weakest assumption since the Otto cycle assumes constant volume heat addition at top dead centre (TDC) when in actual fact combustion starts to take place a few CA before top dead centre (BTDC) to achieve peak pressures around 15CA ATDC and therefore does not take place at a fixed volume. (Milton Brian E., 1995)

3. Isentropic expansion is a weak assumption since combusted fluids are likely to be in a temperature range of 800°C to 2000°C against a significantly cooler cylinder wall and therefore significant heat transfer might possibly occur. (Milton Brian E., 1995)

4. Heat rejection is (in a real engine) takes place by exhaust gases rapidly escaping aided by pressure waves as the exhaust valve(s) open a few CA BTDC, this is known as blowdown. Heat rejection at constant volume is a reasonable approximation to this as during steady state running. (Milton Brian E., 1995)

For the Otto cycle, compression and expansion ratios are equal to:

$$r = \frac{v_1}{v_2} = \frac{v_4}{v_3}$$

Assuming adiabatic compression ( $q = 0; w = du$ ):

$$w_c = c_v(T_1 - T_2) \quad (11)$$

Assuming adiabatic expansion ( $q = 0; w = du$ ):

$$w_e = c_v(T_3 - T_4) \quad (12)$$

Assuming constant volume combustion / heat addition ( $w = 0; q = du$ ):

$$q_a = c_v(T_3 - T_2) \quad (13)$$

Assuming constant specific heats throughout the cycle, combining (11) to (13), (2) and (5) gives thermal efficiency as:

$$\eta_{TH} = \frac{(T_3 - T_4) + (T_1 - T_2)}{(T_3 - T_2)}$$

Simplifying:

$$\eta_{TH} = 1 - \frac{T_4 - T_1}{T_3 - T_2}$$

Since compression and expansion are also isentropic processes:

$$T_2 = T_1 r^{\gamma-1}$$

$$T_3 = T_4 r^{\gamma-1}$$

Substituting and thus simplifying the thermal efficiency  $\eta_{TH}$  for the air standard Otto cycle as a function of compression ratio  $r$  and the isentropic index  $\gamma$  gives:

$$\eta_{TH} = 1 - \frac{1}{r^{\gamma-1}} \quad (14)$$

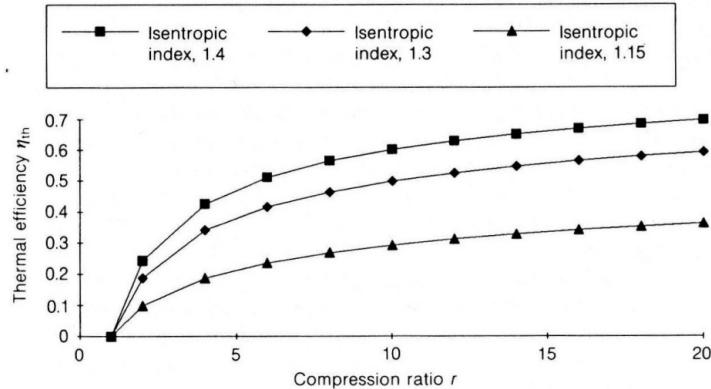
From (14) and a plot of thermal efficiency  $\eta_{TH}$  against compression ratio  $r$  for different isentropic  $\gamma$  values (shown in Figure 5), it can be shown that thermal efficiency is increased by increasing both the isentropic index and the compression ratio.

The isentropic index is not a variable that can be easily changed by the engineer as it is a chemical related property.

In real engines, due to the inevitable heat loss, the compression/expansion stroke is likely to behave like a quasi-adiabatic polytropic process. This implies that the polytropic index will be close to, but less than, the isentropic index, further reducing the thermal efficiency of the engine.

However the compression ratio is a variable that is in the control of the engineer designing the engine. It can be seen that the efficiency will increase infinitely with an infinite increase

in compression ratio. However the rate of increase of efficiency is reducing with the increase of compression ratio. This is to say that the thermal efficiency gains from the increase in compression ratio are not as significant, the higher the compression ratio is.



**Figure 5 - Thermal Efficiency Variation of Otto Cycle (Milton Brian E., 1995)**

Raising the compression ratio sufficiently causes heat transfer out of the system and frictional losses to negate the thermodynamic benefit of such a high compression ratio. It was shown from the work of D.F. Caris and E.E. Nelson, General Motors (GM) that for the combustion chamber they used in their investigation, the optimum compression ratio was 17:1 but was however limited to 10:1 due to engine knock. Recent work shows that the high compression ratios (closer to the optimum) are achievable through better chamber design and utilising lean operation, smaller chambers with high swirl, lower end-gas temperatures to improve knock resistance and better fuels. (Milton Brian E., 1995)

## 2.4.2 Diesel Cycle

The original engine concept of Rudolf Diesel was one which assumed as a constant temperature heat addition to achieve a cycle closer to that of the Carnot cycle and therefore approach the efficiency of the Carnot cycle. In practice a high speed (500-5000rpm) CI engine is actually fairly similar to an SI engine and hence is better matched by the air standard Otto cycle.

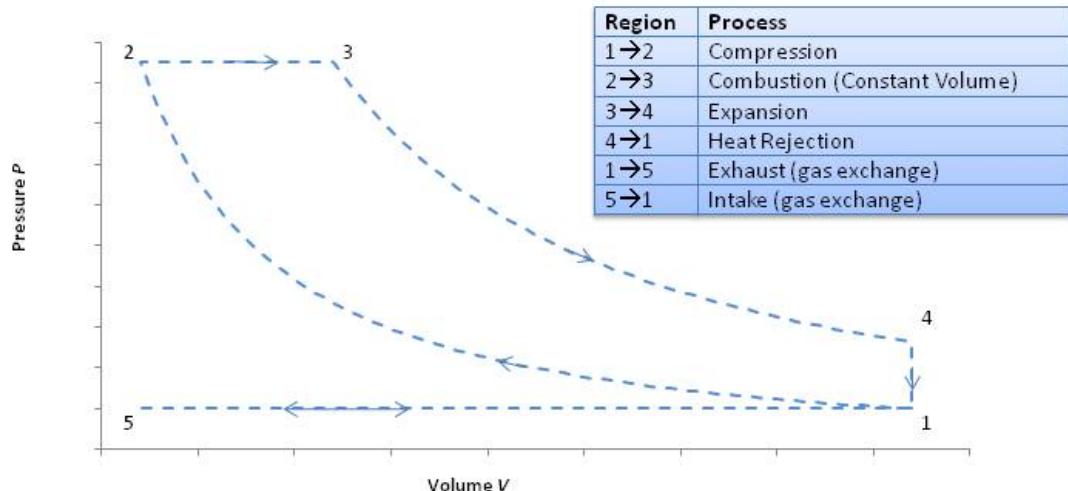


Figure 6 - Air Standard Diesel Cycle

Diesel cycle processes (ignoring gas exchange):

- $1 \rightarrow 2$  Isentropic compression from the initial condition (air in the cylinder at the end of the intake)
- $2 \rightarrow 3$  Constant pressure heat addition
- $3 \rightarrow 4$  Isentropic expansion of the heated gas to produce work
- $4 \rightarrow 1$  Constant volume heat rejection to atmosphere

Therefore the cycle is identical to the Otto cycle with the exception of the heat addition which is assumed to be at constant pressure as opposed to constant volume.

The constant pressure heat addition, the expansion and compression processes occur over different volume ratios defined as follows.

Compression ratio of:

$$r = \frac{v_1}{v_2}$$

Cut-off ratio (volume ratio during heat addition):

$$r_c = \frac{v_3}{v_2}$$

Expansion ratio of:

$$r_e = \frac{v_4}{v_3}$$

The compression is still adiabatic and therefore unchanged from (11) for the Otto cycle. Heat addition is at constant pressure:

$$q_a = c_p(T_3 - T_2)$$

But since  $\gamma = c_p/c_v$  the heat addition is better written as:

$$q_a = \gamma c_v(T_3 - T_2) \quad (15)$$

The compression stroke is identical to that of the Otto cycle in (11). However the expansion is split into two regions. The first part of the expansion stroke is [1] a constant pressure expansion:

$$w_{e1} = p_2(V_3 - V_2)$$

Since  $w = q - du$  from (1) then the expansion work  $w_{e1}$  may be written solely in terms of temperature as:

$$w_{e1} = c_p(T_3 - T_2) - c_v(T_3 - T_2)$$

$$w_{e1} = \gamma c_v(T_3 - T_2) - c_v(T_3 - T_2)$$

The second part of the expansion stroke is [2] an adiabatic isentropic expansion, therefore  $w = q$  giving:

$$w_{e2} = c_v(T_3 - T_4)$$

Therefore the complete work done during expansion  $w_e$  may be written as:

$$w_e = \gamma c_v(T_3 - T_2) - c_v(T_3 - T_2) + c_v(T_3 - T_4)$$

Thus defining the net work  $w_n$  as:

$$w_n = \gamma c_v(T_3 - T_2) - c_v(T_3 - T_2) + c_v(T_3 - T_4) + c_v(T_1 - T_2)$$

Simplifying to:

$$w_n = \gamma c_v(T_3 - T_2) + c_v(T_1 - T_4)$$

Substituting in (5) and simplifying, gives thermal efficiency as:

$$\eta_{TH} = \frac{w_n}{q_a} = 1 - \frac{(T_4 - T_1)}{\gamma(T_3 - T_2)}$$

Given that:

$$\frac{T_2}{T_1} = r^{\gamma-1}, \frac{T_3}{T_2} = r_c, \text{ and } \frac{T_4}{T_3} = \left(\frac{r_c}{r}\right)^{\gamma-1}$$

Thus simplifying to:

$$\eta_{TH} = 1 - \frac{1}{r^{\gamma-1}} \left[ \frac{r_c^\gamma - 1}{\gamma(r_c - 1)} \right] \quad (16)$$

It can be seen from (16) that the thermal efficiency of the Diesel cycle also depends on the cut-off ratio (as well as the compression ratio and isentropic index as was the case in the Otto cycle). However in this case, a higher cut-off ratio reduces the thermal efficiency as can be seen in Figure 7.

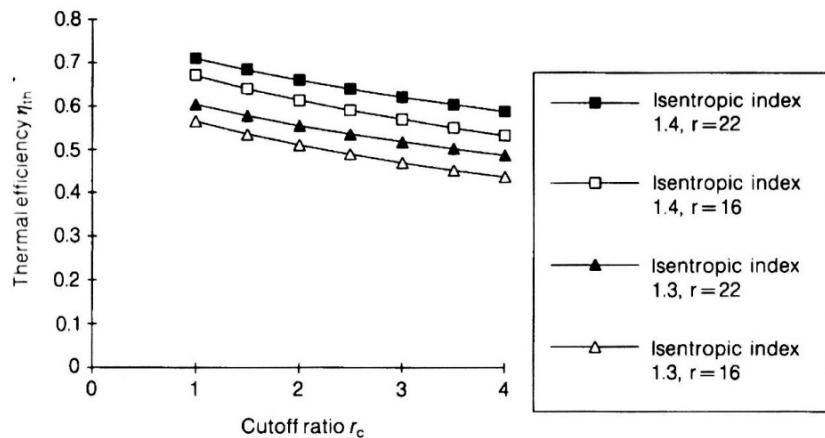


Figure 7 - Thermal Efficiency against Cut-off Ratio (Milton Brian E., 1995)

It is worth considering the squared term in isolation (referred to as the cut-off ratio function) to understand the implications of the cut-off ratio.

$$f(r_c) = \left[ \frac{r_c^\gamma - 1}{\gamma(r_c - 1)} \right] \quad (17)$$

It can be seen that as the cut-off ratio function (17) approaches unity, the thermal efficiency resembles that of the Otto cycle (14), it may also be seen in Figure 8 that the Otto thermal efficiency is achieved when the cut-off ratio approaches unity.

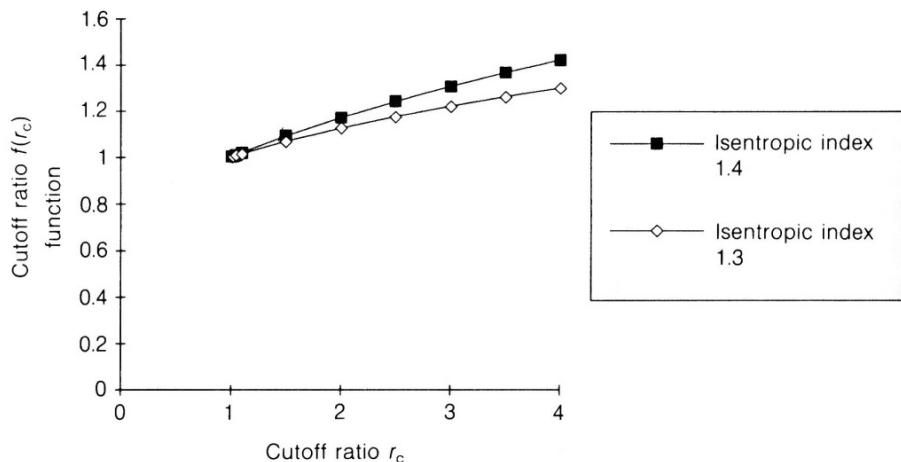


Figure 8 - Cut-off Ratio Function versus Cut-off Ratio (Milton Brian E., 1995)

### 2.4.3 Comparison

Therefore the existence of the cut off ratio clearly indicates a reduction of thermal efficiency of the Diesel cycle when compared to the Otto cycle. This is apparently contradictory to the commonly associations of CI with the Diesel cycle and the SI with the Otto cycle since CI engines are often believed to have a higher thermal efficiency due to their apparent better fuel economy.

In actual fact, an increased cut-off ratio reduces the thermal efficiency, although it does however produce a greater work output. This is made very clear from a pressure-volume diagram (also referred to as an indicator diagram). (Milton Brian E., 1995)

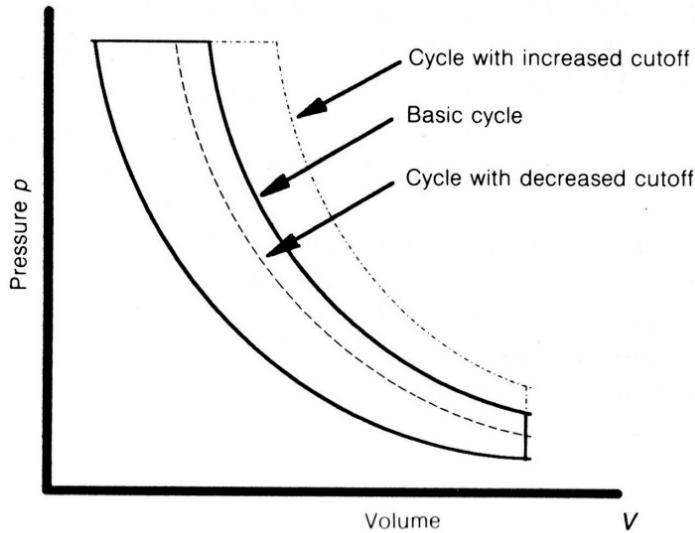


Figure 9 - Cut-off Ratio Effect (Milton, Brian E., 1995)

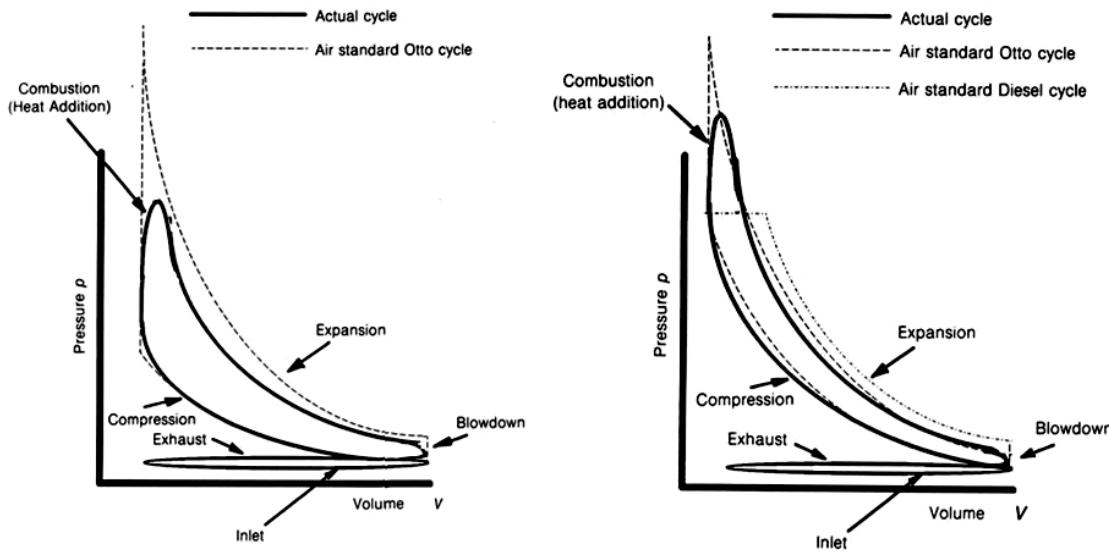
In actual fact, a CI engine is not knock-limited during compression, since the fluid being compressed is air. The ability to run higher compression ratios than the Otto cycle gives a higher thermal efficiency. (Stone, Richard, 1999)

Furthermore, varying the cut-off ratio is a means of controlling the engine load/work output. This is what gives the CI engine the economy advantage over the SI engine in part load conditions. (Milton Brian E., 1995)

CI engines are said to be quality governed, where the amount of fuel is varied and hence varies the fuel/air ratio such as to alter the 'cut-off ratio'. A SI engine is quantity governed, where the air is varied together with the required variation of fuel to maintain a near constant fuel/air ratio (since gasoline has a narrow flammability limit) usually by means of a butterfly valve, resulting in a variation of pumping loss. (Milton Brian E., 1995)

Nonetheless with modern direct injection and stratified strategies for part-load on SI engines, SI technology is behaving similar to CI engines brining reaping their advantages. Similarly CI engines are becoming lighter and more efficient through modern design and manufacturing techniques of combustion chamber design and better light-weight materials are constantly being developed.

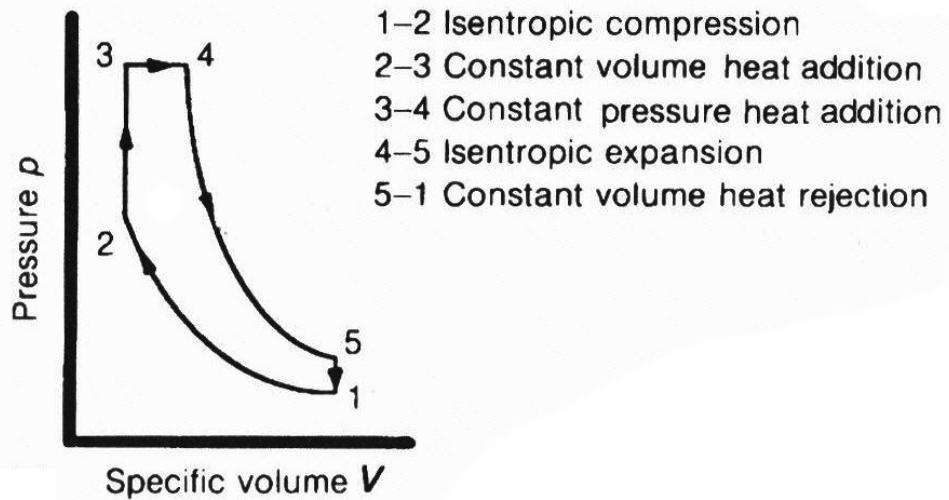
The similarity between technologies is also clear when looking at real indicator diagrams of SI and CI engines. In actual fact none of the two types of engines clearly follow the Otto cycle or the Diesel cycle. This may be seen in Figure 10.



**Figure 10 - Comparison of Indicator Diagrams, Left: SI; Right: CI (Milton Brian E., 1995)**

Since combustion in a SI takes place over a period as opposed to constant volume combustion, the Otto cycle overestimates the peak pressure. The time to fully combust the fuel gives the effect of a cut off ratio. Combustion for the CI engine is slower than that in a SI (due to mixing and diffusion controlled burning in CI), so its reluctance to give a peaky pressure variation is not as bad as the Diesel cycle might suggest.

It is clear that modern SI and CI engines actually behave similar to a cycle that involves part constant volume combustion and part constant pressure combustion. Different variations exist, but the closest (and simplest) standard model that is a cross between the Otto and Diesel cycle is the air standard dual cycle (as shown in Figure 11).



**Figure 11 - Air Standard Dual Cycle (Milton Brian E., 1995)**

## 2.5 Improved Models

From the previous analysis, there are some common gross assumptions leading to considerable discrepancies between standard cycles and real engines, and therefore need to be corrected by further thermodynamic detail, chemical composition and/or phenomena models.

The areas that have been focused in this study:

- Gas Properties – So far the working fluid has been assumed to work as a perfect gas. More detail of thermodynamic properties for (Milton Brian E., 1995 and Heywood, John B., 1988)
- Heat Addition – So far heat addition has been assumed to be an external source, when in actual fact it is an internal combustion. This also occurs over a finite time and volume difference. (Stone, Richard, 1999)

Other areas have been identified (and listed below) but which have not been dealt with in this study. Such areas are:

- Heat transfer in internal combustion engines. Heat transfer is still very poorly understood according to Stone, Richard (1999). Empirical correlations do exist, such as that of Eichelberg developed in 1939 as shown below (in W/m<sup>2</sup>) (Stone, Richard, 1999):

$$\frac{Q_s}{A_s} = 2.43v_p^{\frac{1}{3}}(pT)^{\frac{1}{2}}(T - T_s)$$

- Gas exchange – The gas exchange has been ignored as it has been assumed to produce no pressure drop. This is untrue and pumping losses are of concern at part load when some pressure drop might be expected, in particular when throttling is often applied. (Milton Brian E., 1995)
- Heat Rejection – This has been considered to be at constant volume to the environment as opposed to a blow-down and exhaust stroke. (Stone, Richard, 1999)

### 2.5.1 Working Fluid Properties

In the analysis so far done on the Otto and Diesel cycle so far, it has been assumed that the working fluid throughout the complete cycle may be treated as an ideal gas and with constant specific heats.

Although in actual fact, not only do the properties vary with temperature, the composition of the gas itself also varies through different parts of the cycle (due to external influences, like the addition of fuel, change in temperature, change in pressure and due to chemical reactions).

Process	Spark-ignition engine	Compression-ignition engine
Compression	Air	Air
	Fuel	Recycled exhaust
	Recycled exhaust	Residual gas
	Residual gas	
Expansion	Combustion products	Combustion products

Table 1 - Working Fluid Composition

Table 1- Outlines the working fluid considered in SI and CI. This view in agreement with Heywood, John B. (1988)

	Unburned mixture	Burned mixture
1	Single ideal gas with constant properties (as used in previous cycle analysis)	
2	Ideal unburned gas with unburned properties	Ideal burned gas with burned properties
3	Frozen mixture of unburned ideal gas properties as function of temperature	Frozen mixture of burned ideal gas properties as function of temperature
4	Frozen mixture of unburned ideal gas as function of temperature	Thermodynamic properties based on approximate chemical equilibrium
5	Frozen mixture of unburned ideal gas as function of temperature	Thermodynamic properties based on chemical reaction rates

Table 2 - Models for Predicting Thermodynamic Properties

In agreement with Heywood, John B. (1988), the types of models for predicting thermodynamic properties may be categorised as show in Table 2. For all models, any fuel is treated as a gas. Real gas mixtures may contain large proportions of fuel in vapour form; however the mixture properties are not so easily calculated (Milton Brian E., 1995) and require more complex calculations to determine, and for this reason Heywood, John B.'s distinction for Table 1 has been omitted.

### 2.5.2 Single Ideal Constant

Assuming a single ideal gas, the temperature change may be calculated using the isentropic equations for a volume change during steps  $i$  to  $i + 1$ :

$$T_{i+1} = T_i \left( \frac{v_i}{v_{i+1}} \right)^{\gamma-1} \quad (18)$$

Thus the pressure at state  $i + 1$  may be calculated from the ideal gas law relations as:

$$p_{i+1} = \frac{p_i V_i}{T_i} \left( \frac{T_{i+1}}{V_{i+1}} \right) \quad (19)$$

Modelling (18) would complicate the addition of a burning model in later stages. The temperature change could be calculated as a first estimate as a constant pressure compression/expansion given that the change in volume is small enough. Ackerman, M. (2009). The method is show below (20) to (24).

From (1) for an adiabatic compression/expansion without combustion  $dQ = 0$ :

$$-W = dU \quad (20)$$

Work done during constant pressure compression/expansion:

$$W = p\Delta V \quad (21)$$

Change of internal energy for mass  $m_c$ :

$$dU = m_c c_v (T_{i+1} - T_i) \quad (22)$$

Therefore combining (20) to (22) and re-arranging as:

$$T_{i+1} = T_i - \frac{p(V_{i+1} - V_i)}{m_c c_v} \quad (23)$$

The addition of a burning model would vary equation (23) as (with  $Q = \eta_c m_f h_f \Delta x_b$ ):

$$T_{i+1} = T_i - \frac{p(V_{i+1} - V_i) + \eta_c m_f h_f \Delta x_b}{m_c c_v} \quad (24)$$

Where  $\Delta x_b$  is the mass fraction of fuel burnt (values of 0 to 1) and  $h_f$  is the specific lower heating value of the fuel and  $\eta_c$  is the combustion efficiency. The pressure may then be calculated using (19).

However, the author found that error is significant when either the rate of temperature (and hence pressure) rise/drop is large and/or the piston is an appreciable distance away from bottom dead centre BDC or TDC (since for an equivalent change in CA, the change in volume may not be as small). When combustion occurs, the temperature (and hence pressure) rise is expected to be rapid and therefore the solution is more prone to error. Since the calculated temperature is a value used for further calculations (such as specific heats), it is important to minimise this error as it might be carried over into further calculations, possibly causing overall errors to become more significant.

Using the values obtained for a complete cycle using the above methods as a first approximation, work may now be used to redefine the work done as:

$$W = \frac{p_i + p_{i+1}}{2} (V_{i+1} - V_i) \quad (25)$$

The error may be calculated by re-writing the first law of thermodynamics (1) as:

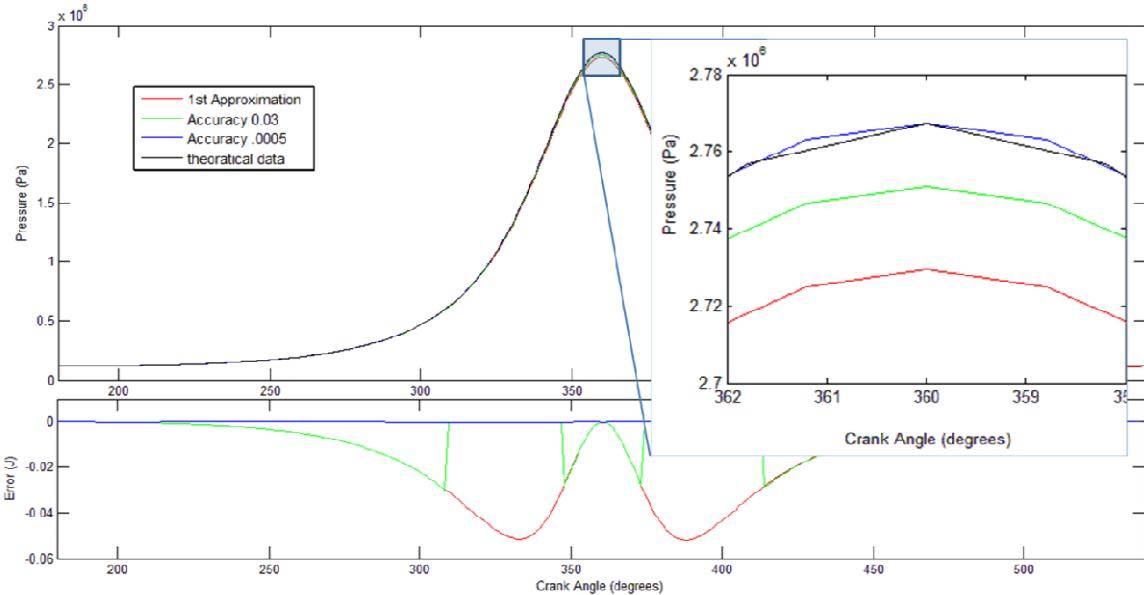
$$E = dU + W - Q \quad (26)$$

The right hand side should evaluate to zero, however since most of the terms are just approximations,  $E$  will be considered the error value re-balancing the equation. Applying the Newton-Raphson (as shown by Stone, Richard, 1999, and Rowland S. Benson and N. D. Whitehouse, 1979), the corrected value of  $T_{i+1}$  for the  $n + 1$  iteration may be evaluated by:

$$(T_{i+1})_{n+1} = (T_{i+1})_n - \frac{E_{(T_{i+1})_n}}{\left(\frac{dE}{dT}\right)_{(T_{i+1})_n}} \quad (27)$$

Having calculated the new temperature,  $T_{i+1}$ , it would then be possible to recalculate any necessary variables (such as specific heats) and thus the pressure  $p_{i+1}$ .

By iterating this method, and establishing a desirable maximum error, a fast converging solution may be obtained with better accuracy than the first approximation.



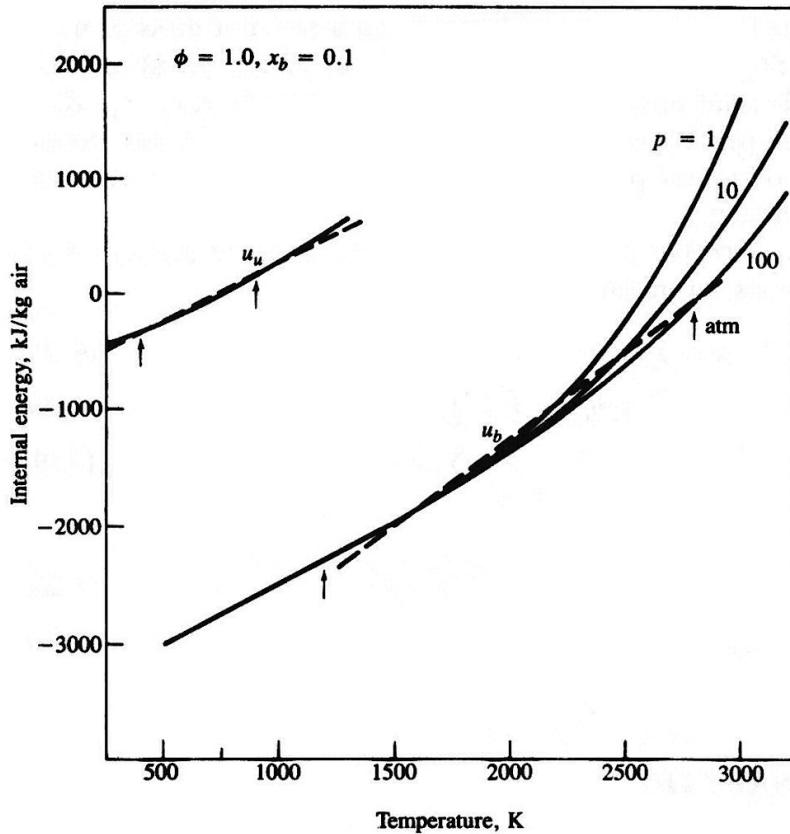
**Figure 12 - Error and Newton-Raphson Method Improvement for a Motored Simulation**

Figure 12 shows a comparison of Pressure against CA and Error against CA. All the values are based on constant thermodynamic properties. The theoretical data is based on first principles of isentropic processes for which the pressure may be calculated exactly. The first approximation and Netwton-Raphson methods of accuracy 0.03 and 0.005 are then compared. The first approximation shows its highest error in the regions 310 to 340CA and 380 to 410CA, this is where it is expected that the volume changes are greater for a given change in CA. However when comparing the iteration producing an accuracy of 0.005, the data is practically identical to the original theoretical data.

### 2.5.3 Idealised Gas Properties

Thermodynamic properties of unburned and burned mixtures may be assumed constant for specific temperature ranges. Figure 13 shows how the specific heat at constant volume (given by (28) may be considered as a constant over specific temperature ranges.

$$c_v = \frac{du}{dT} \quad (28)$$



**Figure 13 - Internal Energy against Temperature for a Stoichiometric Mixture (Heywood, John B., 1988)**

Such graphs are available in existing literature for specific fuels at different fuel to air ratios. It can be shown that fitting a best fit straight line between 1200K and 2800K for the burned mixture is a reasonable approximation. It is important to note that below 1750K the internal energy of the burned mixture is a function of temperature only while above this temperature, the internal energy of the burned mixture is also a function of pressure. (Heywood, John B., 1988)

If considering a burning model producing mass fraction burned  $x_b$ , it is then also used as a blending ratio for unburned and burned properties thus modifying (23) to:

$$T_{i+1} = T_i - \frac{p(V_{i+1} - V_i)}{m_c(c_{v,u}(1 - x_b) + c_{v,b}x_b)} \quad (29)$$

And similarly modifying (24) to:

$$T_{i+1} = T_i - \frac{p(V_{i+1} - V_i) + \eta_c m_f h_f \Delta x_b}{m_c(c_{v,u}(1 - x_b) + c_{v,b}x_b)} \quad (30)$$

### 2.5.4 Frozen Mixture Properties

For models of type 3 to 5 the following formulae are necessary to calculate the properties of mixtures (Ackerman, M., 2009).

The molar fraction of component  $\tilde{x}_i$  for  $n_i$  kmol in mixture of  $n_t$  kmol is defined as:

$$\tilde{x}_i = \frac{n_i}{n_t} \quad (31)$$

The mass fraction of component  $x_i$  for  $m_i$  kg in mixture of  $m_t$  kg is defined as:

$$x_i = \frac{m_i}{m_t} \quad (32)$$

Where the mass of  $m_i$  of  $n_i$  kmol of molecular weight  $M_i$  is given by:

$$m_i = n_i M_i \quad (33)$$

Therefore the molecular weight  $M$  (kg/kmol) of the mixture is given by:

$$M = \sum \tilde{x}_i M_i \quad (34)$$

From the molecular weight  $M$  the specific gas constant  $R$  may then be calculated using the universal gas constant  $\tilde{R}$  as:

$$R = \frac{\tilde{R}}{M} \quad (35)$$

The mixture properties (specific heat at constant pressure and specific heat at constant volume) may be calculated on a molar or mass basis (Heywood, John B., 1988):

$$c_v = \sum x_i c_{v,i} \text{ or } \tilde{c}_v = \sum \tilde{x}_i \tilde{c}_{v,i} \quad (36)$$

$$c_p = \sum x_i c_{p,i} \text{ or } \tilde{c}_p = \sum \tilde{x}_i \tilde{c}_{p,i} \quad (37)$$

The specific heats are related by the specific gas constant as:

$$R = c_p - c_v \quad (38)$$

As well as by the isentropic constant:

$$\gamma = \frac{c_p}{c_v} \quad (39)$$

Therefore, knowing the specific heat properties of each component in the burnt or unburned mixture may be calculated using the ‘old’ form of the NASA polynomials used to represent JANAF thermodynamic tabulated properties for ideal gas mixtures. (McBride B. J. and Gordon, S., 1971)

The ‘old’ form of the NASA polynomials are the most commonly used and often referred to by Heywood, John B., (1988) and Buttsworth, David R., (2002) as shown:

$$\frac{\tilde{c}_{p,i}}{\tilde{R}} = a_{i,1} + a_{i,2}T + a_{i,3}T^2 + a_{i,4}T^3 + a_{i,5}T^4 \quad (40)$$

A newer form of equation (40) exists, published by the original authors McBride B. J. and Gordon, S., (1996). This newer form uses 7 terms to represent the specific heat. However the author has been unable to acquire any coefficients for this form and was unable to pursue it any further. The new form for the specific heat equation is as:

$$\frac{\tilde{c}_{p,i}}{\tilde{R}} = \frac{a_{i,1}}{T^2} + \frac{a_{i,2}}{T} + a_{i,3} + a_{i,4}T + a_{i,5}T^2 + a_{i,6}T^3 + a_{i,7}T^4 \quad (41)$$

Assuming a composition of the fluid that does not vary for during a process (in the compression stroke and/or in the expansion stroke), (36) and (37) may then be applied to all the species or components for which specific heats may be approximated using (40) and (41).

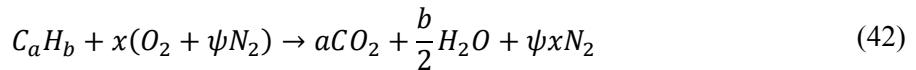
Frozen mixtures may be applied if assuming the reactions are slow enough such that any reactions are negligible. (Heywood, John B., 1988)

### 2.5.5 Approximation of Chemical Equilibrium

From the water-gas equation and equilibrium constants (also known as dissociation constants) for the reactions considered, the moles of products given a known number of moles of reactants.

Equilibrium constants vary with temperature however they may either be assumed constant for a specific temperature range, or they may be calculated from the JANAF tables through look tables or a curve fit.

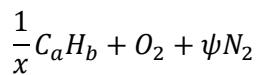
At low temperatures, nitrogen is not considered reactive, and therefore a generic average fuel molecule of  $C_aH_b$  mixed with  $x$  moles of air would oxidise produce complete combustion as (taking air as being made up of 1 mole of diatomic oxygen for  $\psi$  moles of diatomic nitrogen):



Of which the left side are the reactants available and the right hand side are the products. Equating for oxygen implies that the number of moles of air (and hence number of moles of oxygen), gives the air to fuel ratio (AFR), and is shown to be a function of the average number of carbon and hydrogen molecules available in the fuel:

$$x = a + \frac{b}{4} \quad (43)$$

Dividing the reactants from (42) by  $x$ , defines the reactants as fractions per unit quantity on oxygen (or considering each quantity as mole / mole of  $O_2$ ) as:



Separating the above equation per element atom/molecule produces:

$$\frac{a}{x}C + \frac{b}{2x}H_2 + O_2 + \psi N_2$$

Considering a mixture of equivalence ratio  $\phi$  produces so many moles of fuel molecules per mole of oxygen:

$$\phi C_a H_b = \phi \frac{a}{x}C + \phi \frac{b}{2x}H_2$$

Thus re-arranging for the reactants to:

$$\phi \frac{a}{x}C + \phi \frac{b}{2x}H_2 + O_2 \psi N_2$$

Substituting  $x$  with (43) in the above equation produces:

$$\phi \frac{a}{a + \frac{b}{4}}C + \phi \frac{b}{2(a + \frac{b}{4})}H_2 + O_2 \psi N_2$$

Simplifying to:

$$\phi a \left( \frac{4}{4a + b} \right) C + \phi \frac{b}{2} \left( \frac{4}{4a + b} \right) + O_2 \psi N_2$$

If the hydrogen to carbon ratio for the average fuel molecule is defined as:

$$y = \frac{b}{a} \quad (44)$$

Then the reactants may be written as:

$$\phi a \left( \frac{4}{4a + ya} \right) C + \phi \frac{ya}{2} \left( \frac{4}{4a + ya} \right) + O_2 + \psi N_2$$

Further simplifying to:

$$\phi \left( \frac{4}{4 + y} \right) C + \phi 2 \left( \frac{y}{4 + y} \right) + O_2 + \psi N_2$$

$$\phi \left( \frac{4}{4 + y} \right) C + \phi 2 \left( \frac{4 + y - 4}{4 + y} \right) + O_2 + \psi N_2$$

$$\phi \left( \frac{4}{4 + y} \right) C + \phi 2 \left( 1 - \frac{-4}{4 + y} \right) + O_2 \psi N_2$$

Defining the term in the first bracket as:

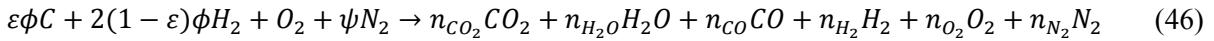
$$\varepsilon = \frac{4}{4 + y}$$

Thus further simplifying the reactants as:

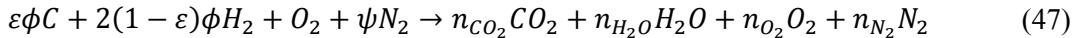
$$\phi\varepsilon C + \phi 2(1 - \varepsilon)H_2 + O_2 + \psi N_2 \quad (45)$$

Equation (45) is useful because all mole quantities are per unit mole of oxygen (reactant). This is the method which Heywood, John B. derives, however this is not the only method. It is known to the author that Turns, Stephen R. (2000) bases the calculations per mole of fuel, which the author found confusing as then the air ratio would then need to be divided by the  $\phi$ , when instinctively,  $\phi$  represents the excess fuel (for  $\phi > 1$ ) for the stoichiometric amount of air.

The products produced by (45) may be written as unknown number of mole/mole of oxygen for each expected product species.

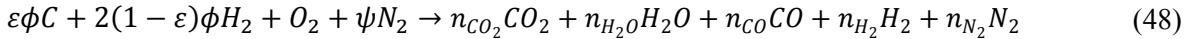


Taking the lean case where  $\phi \leq 1$ , it is reasonable to assume there would be abundant oxygen  $O_2$  to combine with the available hydrogen and carbon molecules and the combustion would therefore not produce any carbon monoxide  $CO$  and diatomic hydrogen  $H_2$ , given as:



Grouping for each product mole ratio term in (47) and solving simultaneously produces the number of moles of products per mole of oxygen (reactant). The sum of the terms produces the total number of moles, and thus dividing each term by the total number of moles gives the molar ratio for the reactants.

Taking the rich case where  $\phi > 1$ , it is reasonable to assume there would be insufficient oxygen  $O_2$  present in the mixture of reactants.



The number of moles per mole of oxygen (reactant) may not be grouped in (48) as there would be insufficient equations to solve. Thus the water-gas reaction needs to be considered and thus the equilibrium constant (Heywood, John B., 1988 and Stephen N. Turns, 2000):

$$K_p(T) = \frac{n_{H_2O} n_{CO}}{n_{CO_2} n_{H_2}} \quad (49)$$

The equilibrium constant is a function of temperature (Stephen N. Turns, 2000) and thus a curve may be fitted from the JANAF tables (Heywood, John B., 1988), and for the reactions considered in (49), this would be:

$$\ln K_p(T) = 2.743 - \frac{1.761E3}{T} - \frac{1.611E6}{T^2} + \frac{0.2803E9}{T^3} \quad (50)$$

From (50) the equilibrium constant together with (48) and (49) provides a quadratic equation (Heywood, John B., 1988):

$$(K - 1)c^2 - c(K(2(\phi - 1) + \varepsilon\phi) + 2(1 - \varepsilon\phi)) + 2K\varepsilon\phi(\phi - 1) = 0 \quad (51)$$

Solving (51) and considering the negative root which produces positive and hence realistic quantities for products, the number of moles per mole of oxygen (reactant). Thus the products of a burned mixture may be tabulated as shown in Table 3.

	Burned Mixture	
	$\phi \leq 1$	$\phi > 1$
$CO_2$	$\varepsilon\phi$	$\varepsilon\phi - c$
$H_2O$	$2(1 - \varepsilon)\phi$	$2(1 - \varepsilon\phi) + c$
$CO$	0	$c$
$H_2$	0	$2(\phi - 1) - c$
$O_2$	$1 - \phi$	0
$N_2$	$\psi$	$\psi$
<b>Sum</b>	$n_b = (1 - \varepsilon)\phi + 1 + \psi$	$n_b = (2 - \varepsilon)\phi + \psi$

Table 3 - Burned Gas Composition Under 1700K (Heywood, John B., 1988)

The number of moles of fuel is the average mass contained in  $\phi C_a H_b$  per mole of oxygen is the mass of that quantity of fuel divided by the average molecular weight of fuel. The mass of the fuel is given by the amounts of carbon and diatomic hydrogen from (45):

$$\phi\varepsilon C + \phi 2(1 - \varepsilon)H_2$$

Given that the atomic weight of carbon and hydrogen 12g/mol and 1g/mol, it then follows that the mass of  $\phi$  molecules fuel for every molecule of oxygen is:

$$mass_{fuel} = \phi\varepsilon 12 + \phi 2(1 - \varepsilon)2 \quad (52)$$

Simplifying to:

$$mass_{fuel} = 4\phi(1 + 2\varepsilon)$$

Thus the number of moles of fuel per unit mole of diatomic oxygen using (33) is given as:

$$n_{fuel} = \frac{4\phi(1 + 2\varepsilon)}{M_f}$$

Thus the number of moles for each species per mole of diatomic oxygen (reactant) is:

$$n_u = (1 - x_b)(reactant\ mixtures) + x_b(burned\ mixtures)$$

$$(1 - x_b) \left( \frac{4}{M_f} (1 + 2\varepsilon) \phi C_a H_b + O_2 + \psi N_2 \right) + x_b (n_{CO_2} + n_{H_2O} + n_{CO} + n_{H_2} + n_{O_2} + n_{N_2}) \quad (53)$$

Substituting from Table 3 for the lean and for a the rich cases for the burned mixtures and grouping each species produces the following tabulated results as shown below and quoted by Heywood, John B. (1988):

	Unburned Mixture	
	$\phi \leq 1$	$\phi > 1$
$CO_2$	$x_b \varepsilon \phi$	$x_b(\varepsilon \phi - c)$
$H_2O$	$2x_b(1 - \varepsilon)\phi$	$x_b(2(1 - \varepsilon\phi) + c)$
$CO$	0	$x_b c$
$H_2$	0	$x_b(2(\phi - 1) - c)$
$O_2$	$1 - x_b \phi$	$1 - x_b$
$N_2$	$\psi$	$\psi$
$Fuel$	$\frac{4(1-x_b)}{M_f}(1+2\varepsilon)\phi$	
$Sum$	$n_u$	$n_u$

Table 4 - Unburned Mixture Composition (Heywood, John B., 1988)

Having obtained the number of moles of each species per mole of diatomic oxygen in Table 4, dividing each term by the total number of moles (indicated by the sum of the terms), the mole fraction for each species is thus obtained, from which the specific heats of the changing gas may be calculated using (36) and (37).

This form of approximate equilibrium calculation is only correct if the assumption that the reactions occur fast enough that the intermediate states of the reaction produce no significant effect. (Heywood, John B., 1988)

$\Phi$	$\chi_{CO}$			$\chi_{H_2}$		
	Full Equilibrium	Water-Gas Equilibrium <sup>a</sup>	% Difference	Full Equilibrium	Water-Gas Equilibrium <sup>a</sup>	% Difference
1.1	0.0317	0.0287	-9.5	0.0095	0.0091	-4.2
1.2	0.0537	0.0533	-0.5	0.0202	0.0203	+0.5
1.3	0.0735	0.0741	+0.8	0.0339	0.0333	-1.8
1.4	0.0903	0.0920	+1.9	0.0494	0.0478	-3.4

Table 5 - Difference between Full and Water-Gas Equilibrium (Turns, Stephen R., 2000)

Table 5 shows the percentage difference between the mole fractions for CO and H<sub>2</sub> at different equivalence ratios when comparing the full and water-gas equilibrium for C<sub>3</sub>H<sub>8</sub>-air at P=1atm. Even though the percentage differences are all below 4% for the example shown, this is not to say that specific heat properties would not vary significantly.

## 2.5.6 Chemical Reaction Rates and Full Equilibrium

The previous method of approximate equilibrium is useful as it gives an indication of the way in which the gas composition and its properties are inclined to change. However as Heywood, John B. (1988) and Turns, Stephen R. (2000) both point out, several other more reactions including the Zeldovich mechanisms for NO<sub>x</sub> formation. Which thus require not only the consideration of more reaction process (besides the water-gas shift) but also the reaction rate and hence the rate of formation. Furthermore, the fast transient nature of internal combustion engines may also cause scenarios where reactions are incomplete due to the gas being cooled sufficiently for the reaction to stop. The lack of consideration for rate of formation and inclusion of minor species in the methods outlined in the previous section, all contribute to a source of error for the varying specific heats of the fluid.

In order to account for all the species that could possibly form, tried and tested ones already exist, such as the NASA Chemical Equilibrium Code developed by McBride, B. J. and Gordon, S., (1971) as well as Olikara and Borman, (1975). Such codes have also been modified and adapted for Matlab by Buttsworth, David R., (2002) and Turns, Stephen R. (2000) and are readily available. These codes are very detailed and have been used by several authors and are therefore considered beyond the scope of the investigation.

Such codes also seem to indicate that when formation rates are of significant importance, the specific heat properties of the mixture do not only depend on its frozen composition at each instant but also has a reaction components (S. Gordon and B. J. McBride, 1971):

$$c_p = c_{p,f} + c_{p,r} \quad (54)$$

Due to the way that the author has built the complete engine model, such auxiliary models may be easily integrated into the code.

Heywood, John B. (1988) and Turns, Stephen R. (2000) both talk about 1500-2000K being the temperature range for which the water-gas equilibrium is sufficient to model the exhaust gases. Appendix B – Validation shows a comparison of the full equilibrium composition at 1750K and the water-gas shift composition for the same said temperature.

## 2.6 Combustion

The energy source that is used to provide heat into the engine and thus providing a gain in net work output is the fuel source. This is combusted by means of a spark or the pressure and temperature conditions due to compression.

In general, IC engines are unable to fully combust the fuel available, resulting in unburned hydrocarbons, and other incomplete combustion products. The measure of efficiency to convert and release the potential fuel energy is referred to as combustion efficiency. (Heywood, John B., 1988; Borman, Gary L. and Ragland, Kenneth W., 1998)

This is often considered to be dependent on the equivalence ratio. The combustion efficiency is considered constant above the maximum-lean limit, producing combustion efficiencies in the regions of 95-98%. In the stoichiometric and rich cases, due to the lack of oxygen, it becomes harder to make full use of the available fuel, producing a considerable drop in fuel combustion efficiency. This is shown in Figure 14. Heywood, John B. (1988) also states that this efficiency is not greatly effected by operating conditions or design variables.

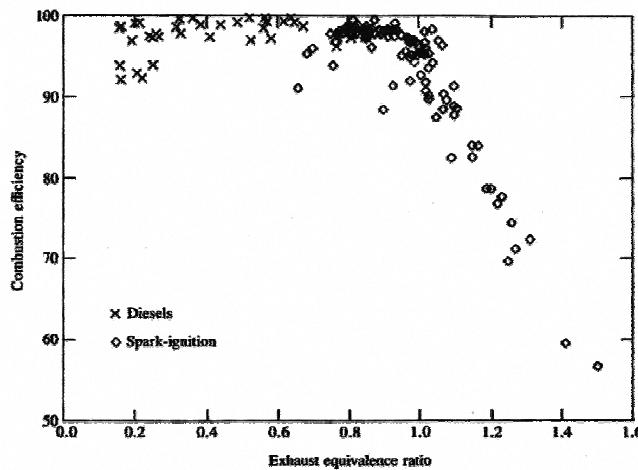


Figure 14 - Combustion Efficiency (Heywood, John B., 1988)

Using the information provided in Figure 14 some piece-wise functions could be defined for combustion efficiency as a function of equivalence ratio. For CI combustion defined as follows in the specified regions (zero elsewhere):

$$f(\phi)_{CI} = \begin{cases} 0.98, & 0.4 \leq \phi \leq 1.0 \\ 0.3\phi + .86, & 0.2 \leq \phi < 0.4 \end{cases} \quad (55)$$

Similarly for SI engines as:

$$f(\phi)_{SI} = \begin{cases} 0.375\phi + 0.6875, & 0.62 < \phi \leq 0.78 \\ 98, & 0.78 < \phi \leq 1 \\ -0.95\phi + 1.93, & 1 < \phi < 1.4 \end{cases} \quad (56)$$

With the limitation of fuel combustion efficiency in mind, the thermal efficiency for a complete cycle may be written as:

$$\eta_{TH} = \frac{W_i}{\eta_c m_f h_f} \quad (57)$$

The equation is similar to those considered for the original standard air cycles, however the heat addition quantity is now limited by the combustion efficiency  $\eta_c$  for the energy in a given mass ( $m_f h_f$ ).

### 2.6.1 SI Homogenous Combustion Modelling

Combustion may occur in two fashions: normal combustion – when combustion occurs at a desired timing through the control of the spark; abnormal combustion – when combustion occurs at undesired timing due to indirectly controlled parameters such as hot spots and excessive gas temperatures and pressures.

For the purpose of this work, only normal combustion is considered, however abnormal combustion is a significant consideration in engine design and control as often causes some deviation from the true desired running conditions of an engine.

Combustion is a three-dimensional, time-dependent, turbulent flow, with a fuel containing blends of different hydrocarbons for which their chemistry is not yet well understood. This could make modelling the combustion process very complex. (Heywood, John B., 1988)

Thus the different approaches need to be considered to establish a desirable level of modelling and detail within the scope of this work. Stone, Richard (1999) outline the following three main categories:

- Zero-dimensional/phenomenological models – Empirical based heat release models. These are independent of time.
- Quasi-dimensional models – These use a turbulent combustion model to derive a heat release model.
- Multi-dimensional models – Numerically solving mass, momentum, energy and species conservation in three dimensions to predict flame propagation.

Multi-dimensional models hint to being an entire study in their own right, requiring the computing of modern CFD codes as well as detailed geometry design, which goes beyond the scope of this work (to easily predict overall performance characteristics from basic engine parameters). (Stone, Richard, 1999)

Quasi-dimensional models require the consideration of burned and unburned gas properties such as their density to be taken separately as well as a laminar flame front making the current modelling approach for most of the mixture properties unsuitable. (Stone, Richard, 1999)

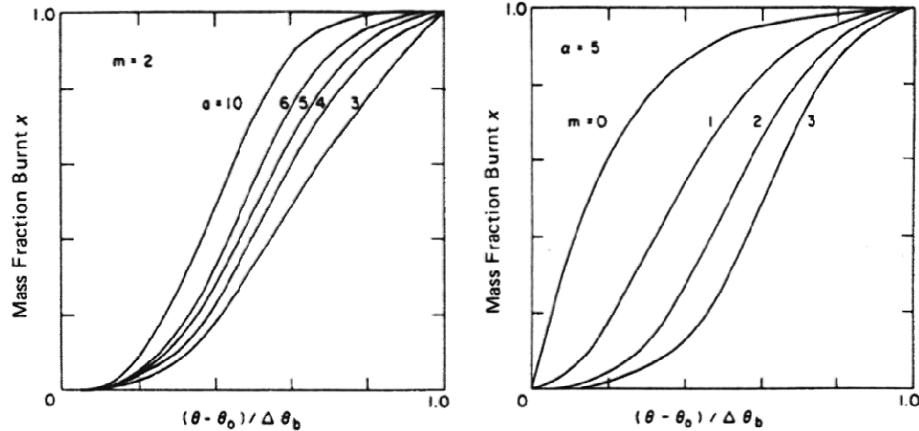
Zero-dimensional/phenomenological models are thus the remaining option with which the author achieved desirable agreement with test data. Furthermore, this is the preferred method to be employed for further emission analyses for the estimated equilibrium thermodynamic properties discussed earlier as well as future possibilities of Zeldovich mechanisms to predict nitric oxide emissions. (Stone, Richard, 1999)

A commonly applied zero-dimensional burning model is the Wiebe (1967) function referred to by Heywood, John B., (1988) and Stone, Richard (1999):

$$x_b(\theta) = 1 - e^{-a\left(\frac{\theta-\theta_0}{\Delta\theta_b}\right)^{m+1}} \quad (58)$$

Where  $\Delta\theta_b$  is the duration in crank angles over which combustion takes place (typical values quoted are 60 to 70 degrees),  $\theta_0$  is the crank angle at which combustion starts, resulting in a mass fraction burnt  $x_b$  at any given crank angle  $\theta$ .

The only two calibration constants are  $a$  and  $m$ , which are often taken to be as 5 and 2 respectively. Their effect on the fraction burn may be shown to be as:



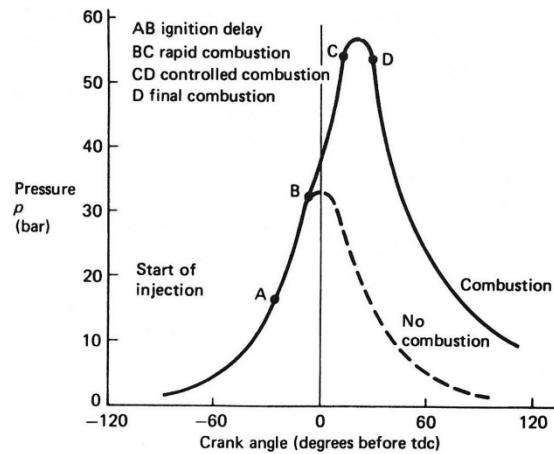
**Figure 15 - Wiebe Functions (Stone, Richard, 1999)**

The combustion progress may be categorized in three regions, an initial flame development region, which often takes place approximately over the first 10% of the duration, followed by rapid-burning process during which the bulk of the mixture is consumed and is seen as a rapid consumption of the unburned mixture, often spanning a further 10% of the duration, with a final slow-burning process in the remaining 10% of the duration. (Heywood, John B., 1988)

Occasionally ignition delay and/or delay period are mentioned in SI engines; however the authors seem in disagreement with the use of such terminology. Heywood, John B. (1988) associates with the initial slow flame development, however counter argues that combustion is almost instantaneous in SI engines and is of only real concern in CI engines.

## 2.6.2 CI Combustion Modelling

Unfortunately the modelling of CI combustion is far less trivial than SI combustion. The lack of a homogenous mixture implies that not all the available gas is in a state capable of maintaining combustion initially.



**Figure 16 - Hypothetical pressure diagram for a CI engine (Stone, Richard, 1999)**

With reference to Figure 16 and Figure 17, the four stages of combustion may be seen and identified. There are the following stages (Heywood, John B., 1988; Stone, Richard, 1999; Ricardo, Harry R. and Hempson, J.G.G., 1968):

- **Ignition delay period (A to B)**

This is the period from the start of injection until the start of combustion during which there is no apparent heat release. This is due to the low volatility of the fuel which is often still in droplet form when first injected. The fuel is then vaporised and mixed with the air until there are regions that have undergone sufficient mixing which will then sustain combustion (some minor reactions would still be occurring during this delay period).

The longer the delay period the higher the pressure peak may be expected as it implies more of the fuel is in the cylinder available for combustion. A control method to attempt to minimise the delay period is a slow fuel delivery in order to wait for the ignition delay period to be over, before all the fuel is present, or through the use of a pilot injection.

- **Rapid/Uncontrolled Combustion/Pre-mixed combustion (B to C)**

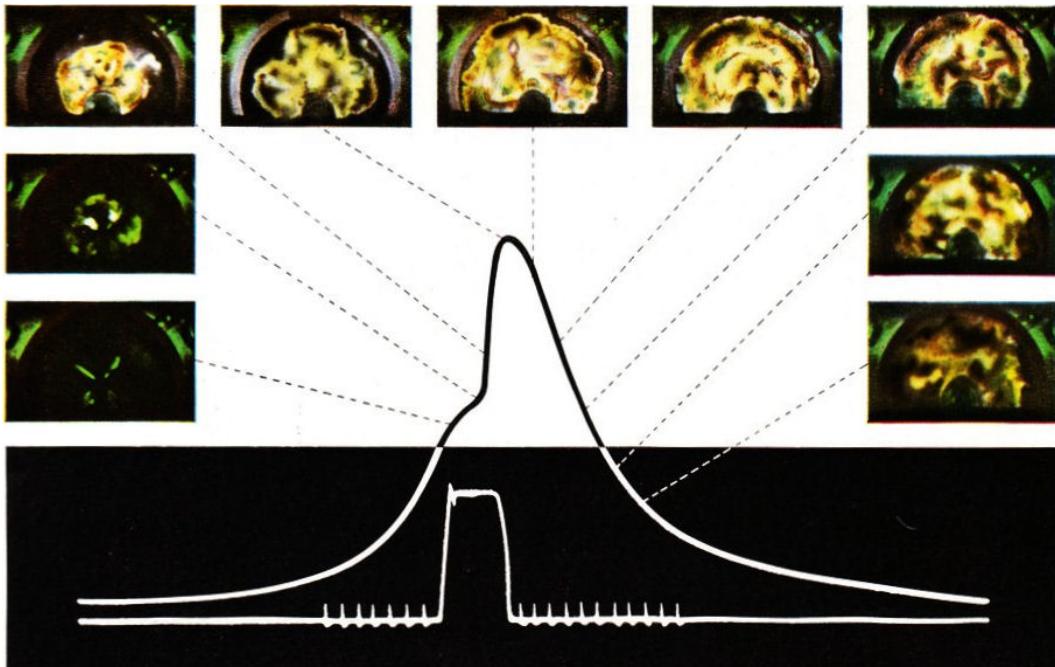
During the ignition delay period an amount of fuel would be readily mixed within flammability limits of fuel-air mixtures and is then readily available for combustion not too dissimilar to that in SI homogenous combustion.

- **Mixing/Controlled Combustion (C to D)**

This is the region in which burn rate is fast as the remaining fuel and air may be mixed into the desired fuel-air mixtures. This part of combustion may cause a second distinct heat release peak (and/or pressure peak).

- **Late combustion phase (D to E)**

Heat release will still take place at lower rates for periods in the expansion stroke. This is due to the minor portions of unburned fuel as well as the soot and fuel-rich combustion products that may still be able to release further energy. This is thus predominantly diffusion controlled and less significant the better the rapid and mixing phases are.



**Figure 17 - Flame Propagation in a CI Engine (Ricardo, Harry R. and Hempson, J.G.G., 1968)**

Modelling of CI is less trivial to model even with a phenomenological model since there are several stages of the complete combustion process, and since most of the processes depend on the ability to vaporise and mix the available fuel and air, it also follows that the chamber and injector design have a greater influence. (Stone, Richard, 1988)

However, an adaptation of the Wiebe model may be used (suggested by Heywood, John B., 1988, and in agreement with Stone, Richard, 1988) if the processes were simplified as:

1. Delay period – treated as a dead period during which no heat release is imitated and is still in droplet form, thus having no practical influence on the properties of the working fluid.
2. Flammable mixture – treated as a pre-mixed rapidly burning quantity controlled by a function.
3. Final/Diffusion combustion – the remaining air to fuel mixed is then burned and controlled by another function (in which mixing controlled and late combustion are in a sense grouped).

Thus the function for predicted mass fraction burn may be defined (as developed by Watson et al. 1981):

$$x_b(\theta') = \beta f_1(\theta') + (1 - \beta)f_2(\theta') \quad (59)$$

Where  $\beta$  is the fraction of fuel burned in the pre-mixed rapid phase,  $f_1(\theta')$  and  $f_2(\theta')$  are the pre-mixed and diffusion burn functions providing the total mass fraction burned  $x_b(\theta')$  at a given instant, where  $\theta'$  is a fraction of the full combustion duration (it should be noted that the duration is considerably longer than that for SI homogenous combustion, often around 120 crank angles, this value is supported by the author's model comparison results as well as the Heywood, John B. (1988)):

$$\theta' = \frac{\theta - \theta_{ign}}{\Delta\theta_{duration}} = \frac{t - t_{ign}}{\Delta t_{duration}} \quad (60)$$

Since typical fuels have this reluctance to readily combust, the greater the ignition delay the less likely the fuel is combusted in the pre-mixed phase (indicating a slow diffusion or poor chamber design. Conversely, a richer mixture increases the likelihood of an ignitable fuel-air mixture to form. However these relationships are not linear or of a calculable form, rather they are based on empirically evaluated constants:

$$\beta = 1 - \frac{a\phi^b}{(t_{id})^c} \quad (61)$$

Where  $t_{id}$  is ignition delay measure in milliseconds (typical of 0 to 2ms at most speeds, but can be higher at low load and low speed conditions) where constants  $a$ ,  $b$  and  $c$  need to be empirically established. Heywood, John B. (1988) quotes a range for these constants for a typical turbocharged diesel engine:

$$0.8 < a < 0.95; \quad 0.25 < b < 0.45; \quad 0.25 < c < 0.5$$

The burning functions are adaptations of the Wiebe function:

$$f_1 = 1 - (1 - \theta'^{K_1})^{K_2} \quad (62)$$

$$f_2 = 1 - e^{-K_3\theta'^{(K_4)}} \quad (63)$$

Where  $K_1$  to  $K_4$  need to be empirically established, Heywood, John B. (1988) quotes:

$$K_1 = 2 + 1.25 \times 10^{-8}(t_{id}N)^{2.4}$$

$$K_2 = 5000$$

$$K_3 = \frac{14.2}{\phi^{0.644}}$$

$$K_4 = 0.79K_3^{0.25}$$

The ignition delay value  $t_{id}$  may also be deducted by two correlations; Stone, Richard (1999) refers to one such method by Watson (1979) relates this parameter to the mean temperature and pressure during ignition delay. While this method is useful as it requires no knowledge of the fuel properties, it does require an iterative approach since the mean temperature and pressure are depending on values that might not have yet been calculated (since they require the burning model).

$$t_{id} = \frac{3.52e^{\frac{2100}{T}}}{p^{1.022}} \quad (64)$$

Heywood, John B. (1988) refers to correlation developed by Hardenberg and Hase (1979), where the fuel Cetane number and engine speed are factored in (and rightly so, since ignition delay varies with how well the fuel can mix which is promoted by the air flow in the chamber), providing a value for the ignition delay in crank angles at a given engine speed:

$$t_{id} = (0.36 + 0.22v_p)e^{E_a \left( \left( \frac{1}{R_0 T} - \frac{1}{17190} \right) \left( \frac{21.2}{p - 12.4} \right) \right)^{0.63}} \quad (65)$$

Where,  $v_p$  is the average piston speed and easily calculated from the engine speed and stroke length,  $T$  and  $p$  are temperature (K) and pressure (bar) respectively at TDC which may be easily estimated by modelling the compression as a polytrophic process.  $E_a$  is a function of the fuel cetane number  $CN$  where  $E_a = \frac{618840}{CN+25}$ .

The evaluation of the ignition delay has not been considered further in this work, other than having visited the available methods of evaluating it to have an understanding of their influential parameters and an appreciation for the magnitude and influence.

Having considered these empirical burning models, the association of the Otto cycle with SI combustion and Diesel cycle with CI combustion is more obvious. Though on first glance CI indicator diagrams tend to indicate a peaky pressure curve, it is misleading, as it does not make it obvious that the fuel is still undergoing combustion for a period of around 120CA, making the constant pressure heat addition assumption more viable than the ‘fast’ constant volume heat addition of the Otto cycle.

However modern CI engines can reach higher speeds, due to their improvements permitting CI fuels to pre-mix and continuing mixing more rapidly. This is owed to the advancements of computer simulation which permit better modelling of spray patterns and flow patterns within the combustion chamber. Nevertheless, significant theory on turbulence modelling is yet unknown.

### **3. Aims of the Investigation**

The aim of the investigation was to:

- Acquire a clear understanding of the thermodynamics and combustion theory available such as to piece it together and develop a set of useful tool set for future work and demonstration of the key fundamentals of internal combustion engines.
- Create a simulation framework to explore and simulate these fundamentals and thus demonstrate the understanding of the said fundamentals.
- Use the simulation to run “what if” scenarios

It was deemed by the author that the tools that were to be developed as a set of modules which when put together may be used to simulate a SI (homogenous) or CI engine. It was preferred to have the least dependence on exact engine geometry knowledge (other than some basic geometric features). With the scope of future proofing and creating a set of the tools that are not very task-specific, it was deemed that a modular modelling approach would provide this:

- To facilitate validating the model either as a whole or in part (based on previous literature or test data)
- To be of possible use for other projects (such as the work of Mark Elliot that requires some pressure and temperature information in order to predict in detail NO<sub>x</sub> emissions)
- To facilitate the addition of future modules (such as one to simulate variable valve timing)

Consideration of the gas exchange might have required further engine geometric detail (cam profiles, valve size, etc) that are not readily available while also making the result harder to validate with the available resources. The following minimum inputs were decided upon for the final iteration of the model:

Engine Geometry: Compression Ratio, Bore Diameter, Rod length and Stroke/Crank Radius

Chemical Properties: Fuel type (and combustion method), Initial Pressure, Initial Temperature and Specific heat properties if opting to assume frozen composition and temperature invariant properties.

Engine Running Conditions: Engine Speed, Equivalence ratio, Ignition Timing, Combustion Duration and Ignition delay (for CI)

The following data outputs were desired (for the complete simulation):

- In cylinder average pressure (against volume/crank angle)
- In cylinder average temperature (against volume/crank angle)
- Work done (excluding pumping losses)
- Thermal efficiency (excluding pumping losses)
- Mass fraction burn

## 4. Investigation & Development

The theory required to develop the final tools have mostly been covered in the literature review, and most of the work discussed here is the final iteration and the final state of the simulation tools since several minor and major changes were made which would be beyond the scope of this work to explain. Nonetheless much of the major conclusions of the major branches down the road to the final set of simulation tools have been documented.

### 4.1 Preliminary Work

Initial theory and understand was tested on MS Excel, as this permitted quick and easy way of verifying understand as one could easily track the numerical progress to a solution.

Possible sources of error:

**A: Combustion pressure**

- Pressure transducer low response
  - Constant volume assumption wrong
- Need to account for burn rate

**B: Higher temperature compression:**

- Adiabatic assumption wrong
- Incorrect gas properties

**C: Lower temperature expansion:**

- Result of instantaneous combustion (A)
- Adiabatic assumption
- Incorrect gas properties

**Other:**

Fluid properties

Fluid composition

Initial conditions

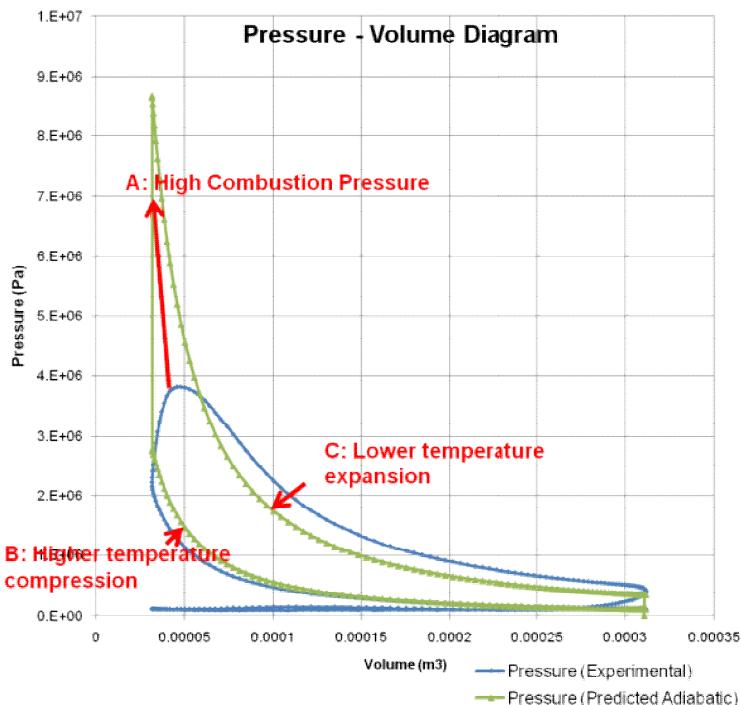


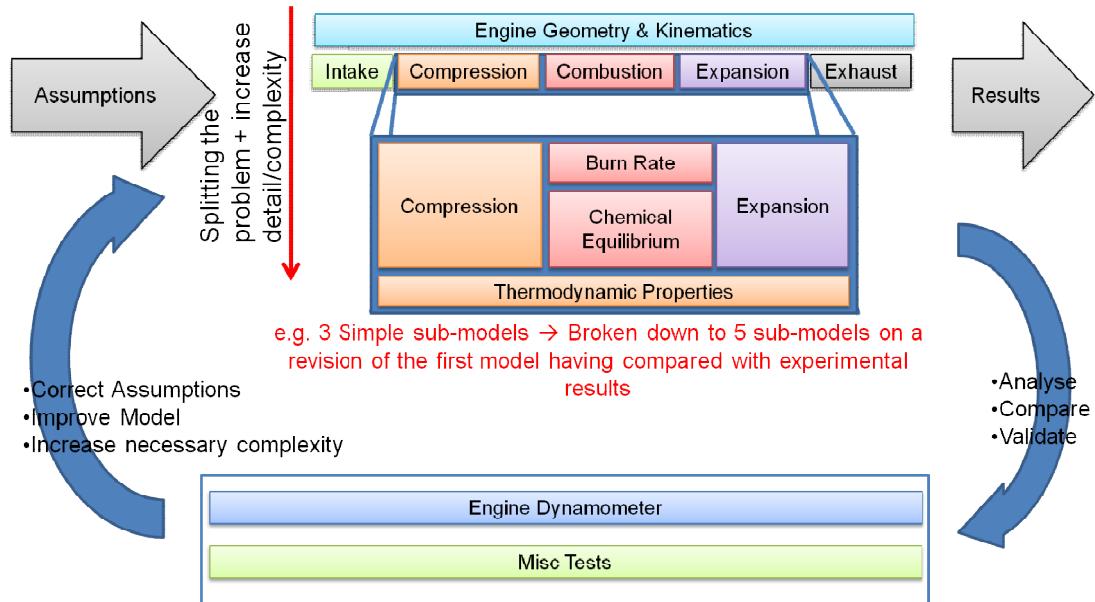
Figure 18 - First Simulation Results and Analysis

Very early on, even when simulating the Otto cycle (as shown above in Figure 18) it was easy to envision the simulation tools growing too complex to contain in MS Excel or to manage and validate with ease. Having had first experience at modelling internal combustion, an outline of the envisioned modelling approach was made that would lead to forming the final simulation tool set.

#### 4.1.1 Modelling Approach

A modelling approach (or even just the awareness of one) was proven crucial; as such an exercise grew in complexity very rapidly and hence would have been hard to develop without identifying the difficulties that would develop ahead.

Assumptions would need to be made for each part of the model. Each part or complete set of models would produce results which would then need to be analysed, compared and validated against tests data, or cited data. The outcome of this would feed to correcting the assumptions, improving the model or further subdividing the model and thus increasing its complexity. This is pictorially further explained in Figure 19.



**Figure 19 - Modelling Approach**

The example demonstrates how a model made of 6 sub model (Engine geometry, Intake, Compression, Combustion, Expansion and Exhaust), may require some of the sub models, to be further broken down (Combustion is now broken down into Burn Rate and Chemical Equilibrium parallel to it) while adding possibly more sub models parallel existing ones (Compression, Burn Rate, Chemical Equilibrium, Expansion now work in parallel with a Thermodynamic Properties sub model).

#### 4.1.2 Choice of Development Method

A number of software packages and languages were available to select from, an evaluation of each was conducted.

Method	Advantages	Disadvantages
Excel	Widely available	Cannot see source of built in calculations
	Easy to use	Can easily over-crowd the screen/spreadsheet
	Well known to the author	Hard to track data flow
	Easy to monitor variables/calculations	Hard to expand
	Platform dependent	Slow to execute
C/C++	Widely available	Requires strong programming knowledge
	High level of control	Might be less useful to others in the future
	Known to the author	Might cause debugging code more than model
	Fast to execute	
	Cross platform compatible	
Matlab	Commonly associated for engineering problems	Not as well known to the author
	Reasonable execution time	Not as readily available as Excel/C/C++
	Has several useful built-in functions	Requires reasonable programming knowledge
	Has some level of cross platform	
	Easy to monitor variables/calculations	
	Easy to track data flow	

**Table 6 - Different Modelling Environments**

Matlab was the preferred option (this was supported by the strong use of this package in industry, deeming any time to spent to learn more on how to use this package as a good investment). Having experienced using several programming languages (including PASCAL, BASIC, C/C++) as well as GUI interfacing (including OpenGL, SDL), learning Matlab was considered as feasible, as it not only provides a framework for engineering problem solving (such as built-in matrix functionality), but many scripts and functions are available to ‘expand’ its purpose.

#### 4.1.3 Validation

Validation was to be done against a number of sources. For the main part of the work, most of the validation would be done against data off the Rover K-Series at UWE. The second source was to be a Ford 2.4L turbo diesel engine which would be fitted onto the most recent dynamometer at UWE which has had a new controller fitted, and for which several new components had to be ordered in and fitted (such as mounting brackets and an aftermarket ECU).

Due to logistical shortcomings from the engine supplier, the engine has only recently been physically mounted. The importance of this engine was necessary for validating fine details of the model. Alternative data from a similar sized diesel engine has been used to interpret the results of this part of the model.

However Mark Elliot was capable of sourcing some pressure readings from a diesel engine whose details may not be disclosed in this work (due to confidentiality issues imposed on the original un-named author).

The other major source of validation was the literature available (in particular for the generic thermodynamic modelling). Please see Appendix B – Validation .

## 5. Simulation

Figure 20 shows the final arrangement chosen by the user for which the Matlab functions are listed in Appendix A – Function List. The green box represents the necessary user inputs to the main engine simulation function represented by the red box, while the blue boxes represent the individual functions that need to be called to output the variables represented by the grey box.

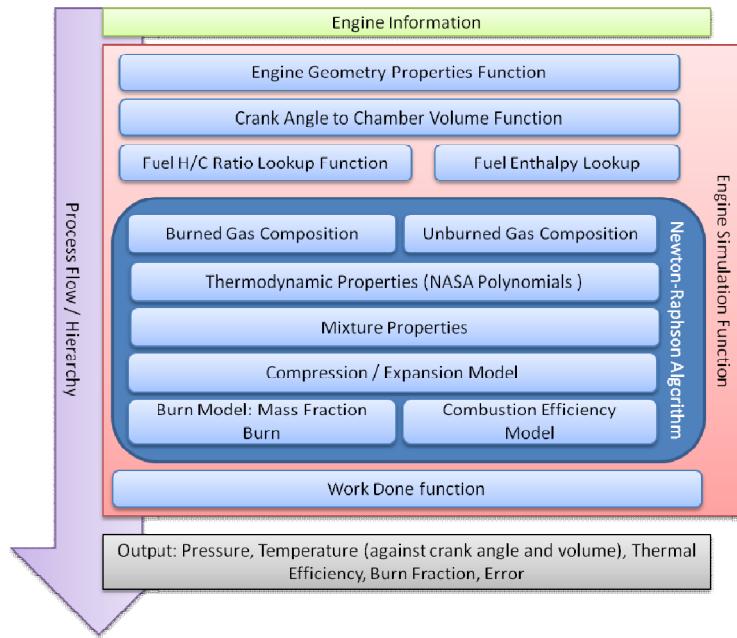


Figure 20 - Process Flow / Hierarchy

Full functionality is available from the command line interface of matlab via the function ESim(...) or via the GUI shown in Figure 21.

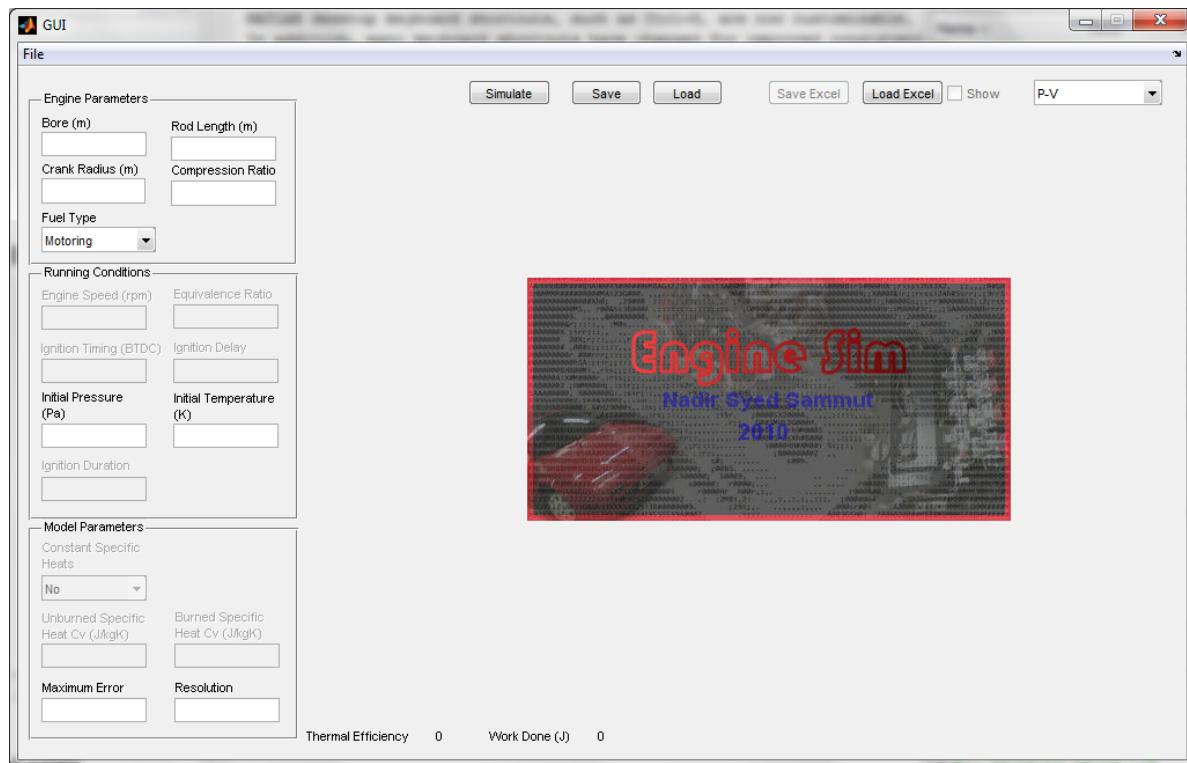


Figure 21 - Engine Sim Interface

Engine Parameters	
Bore (m)	Rod Length (m)
<input type="text"/>	<input type="text"/>
Crank Radius (m)	Compression Ratio
<input type="text"/>	<input type="text"/>
Fuel Type	
Diesel	<input type="button" value="▼"/>
Running Conditions	
Engine Speed (rpm)	Equivalence Ratio
<input type="text"/>	<input type="text"/>
Ignition Timing (BTDC)	Ignition Delay
<input type="text"/>	<input type="text"/>
Initial Pressure (Pa)	Initial Temperature (K)
<input type="text"/>	<input type="text"/>
Ignition Duration	
<input type="text"/>	
Model Parameters	
Constant Specific Heats	
No	<input type="button" value="▼"/>
Unburned Specific Heat Cv (J/kgK)	Burned Specific Heat Cv (J/kgK)
<input type="text"/>	<input type="text"/>
Maximum Error	Resolution
<input type="text"/>	<input type="text"/>

Figure 22 - Available Parameters

The Engine Sim requires the following parameters: Bore, Rod Length, Crank Radius and a Compression Ratio, Initial Pressure, Initial Temperature, a Resolution, Maximum Error.

These parameters may be saved and load via the GUI to facilitate swapping between the various engines.

**N.B. The Resolution field is misleading as what was actually meant is the ‘number of steps’, as opposed to the size of the step, however the term has been kept for consistency within the functions.**

With these basic parameters, a motored (no fuel and thus no combustion) simulation may be run.

Upon changing the fuel type to one of: Gasoline, Iso-octane or Propane; further parameters are required: Engine Speed, Equivalence Ratio, Ignition Timing (BTDC), Ignition/Combustion Duration.

If the fuel type chosen is Diesel, then an ignition delay value is expected.

For the specific heat properties, the user may opt to allow the model to use the specific heat and temperature relationships as well as the exhaust gas composition to calculate the mixture properties.

However the user also has the option to simplify the model to that of the type which assumes a constant specific heat for the unburned mixture and another value for the burned mixture, in which case, they would need to be specified.

Some verification has been implemented to ensure sensible values have been entered, but the verifications are not extensive and do rely on the user understanding the implications of the parameters entered.

The GUI is capable of plotting: P-V, T-V, P-CA, T-CA,  $x_b$ -CA and E-CA graphs. It is also capable of exporting to Excel volume, crank angle and pressure values. There is the option to import volume, crank angle and pressure volumes from Excel with the option to superimpose the data with the simulation results for comparison. This is the method used to draw the overall conclusions.

The specific detail of the programming is not explained here since this was never meant to be a programming exercise. Nonetheless the author had to acquire new programming skills, in particular for the GUI interface. The code is available Appendix A – Function List and on the accompanying CD and due to its modularity, it should be straight forward to at least understand the purpose of each function from the in line comments.

## 6. Results & Conclusions

As mentioned in previous sections, the model was validated as a whole against two sets of data from two different engines. The test data is included as spreadsheets on the accompanying CD. Comparisons have been drawn with the simulation work of Ackerman, M. (2009).

### 6.1 Simulation of SI

Test Data Conditions		Final Simulation Parameters	
Engine:	Rover K-Series 1120cc	Initial Temperature	330 K
Throttle:	100%	Initial Pressure	1.05bar
Ignition timing:	15CA +/- 1CA BTDC	Ignition timing:	15CA BTDC
Engine Speed:	3000rpm	Engine Speed:	3000rpm
Fuel	Pump fuel	Fuel	Gasoline
Equivalence Ratio	~1.0	Equivalence Ratio	0.98
		Ignition Duration	68CA

Ackerman M. (2009) had achieved reasonable agreement in their work using spreadsheet based models, using an initial temperature of 350K and initial pressure of 1.15bar (based on Heywood, John B., 1988's publication). It was later decided that 330K and 1.05bar seemed more likely. The author accepted these values due to Ackerman, M.'s long experience with this specific engine and test facility, as well as a wiser experience in the field.

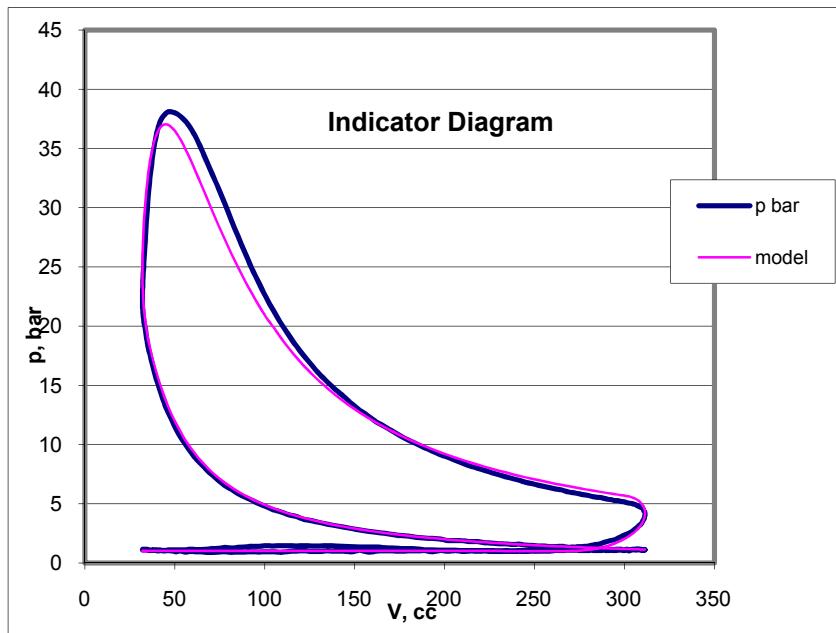


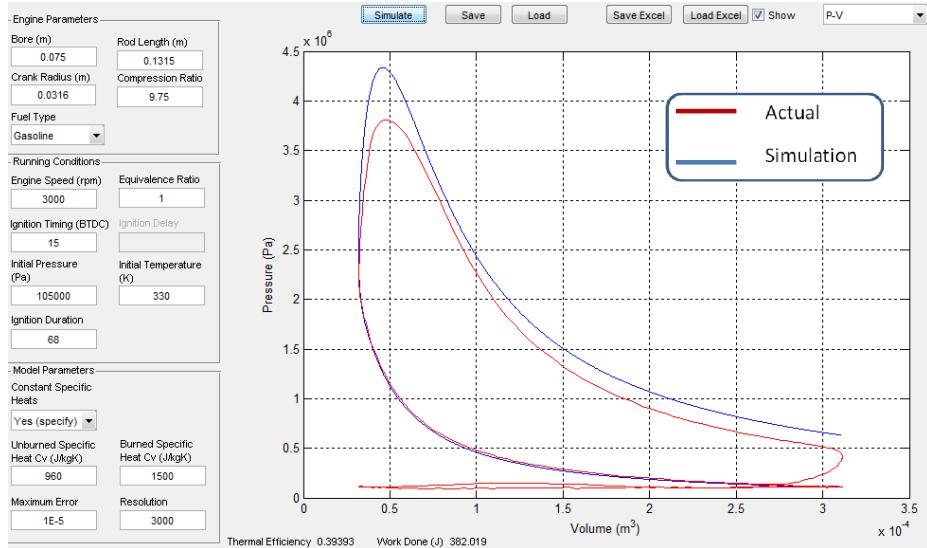
Figure 23 - Indicator Diagram (Ackerman M., 2009)

It was noted that Ackerman M., applied a combustion efficiency of around 80%. The seemed too low since Heywood, John B. states at normal operating fuel-air mixtures, 95-98% combustion efficiency is expected (refer to section 2.6). The author suspects that Ackerman, M., did so perhaps to act as an overall efficiency reduction, however such an addition would falsely hinder the cycle only during the combustion phase, and give a dishonest higher thermal efficiency value.

Since the combustion efficiency variation with equivalence ratio has been incorporated in the author's model, there was no need to consider it while varying running conditions. The

combustion/ignition duration and equivalence ratio were the only two parameters left at the author's disposal to tweak the model parameters.

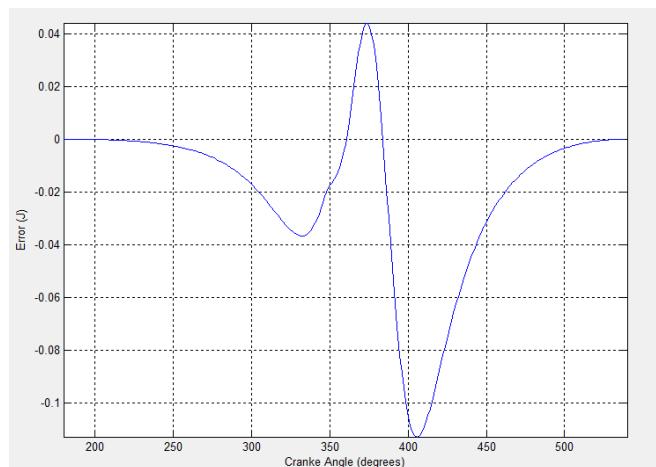
Using the same constant specific heats as in the work of Ackerman, M. (960J/kgK for the unburned mixture and 1500J/kgK for the burned mixture) provided the following result and adjusting the combustion/ignition duration to 68CA (Heywood, John B., 1988, recommended about 70CA):



**Figure 24 - Simulation Comparison with Constant Properties**

The general shape of the indicator diagram was in agreement with that of the data; however the peak pressures and work output were significantly higher than that of the real engine. This is not apparent in Ackerman, M.'s results due to their under-estimation of the combustion efficiency.

Varying the maximum permissible error had minimal effect to the overall shape of the indicator diagram. This is to be expected since constant specific heats are independent of temperature, thus the error of assuming constant pressure expansions to evaluate the temperature at that step, are only carried over to the next step as a false initial condition for the next step.

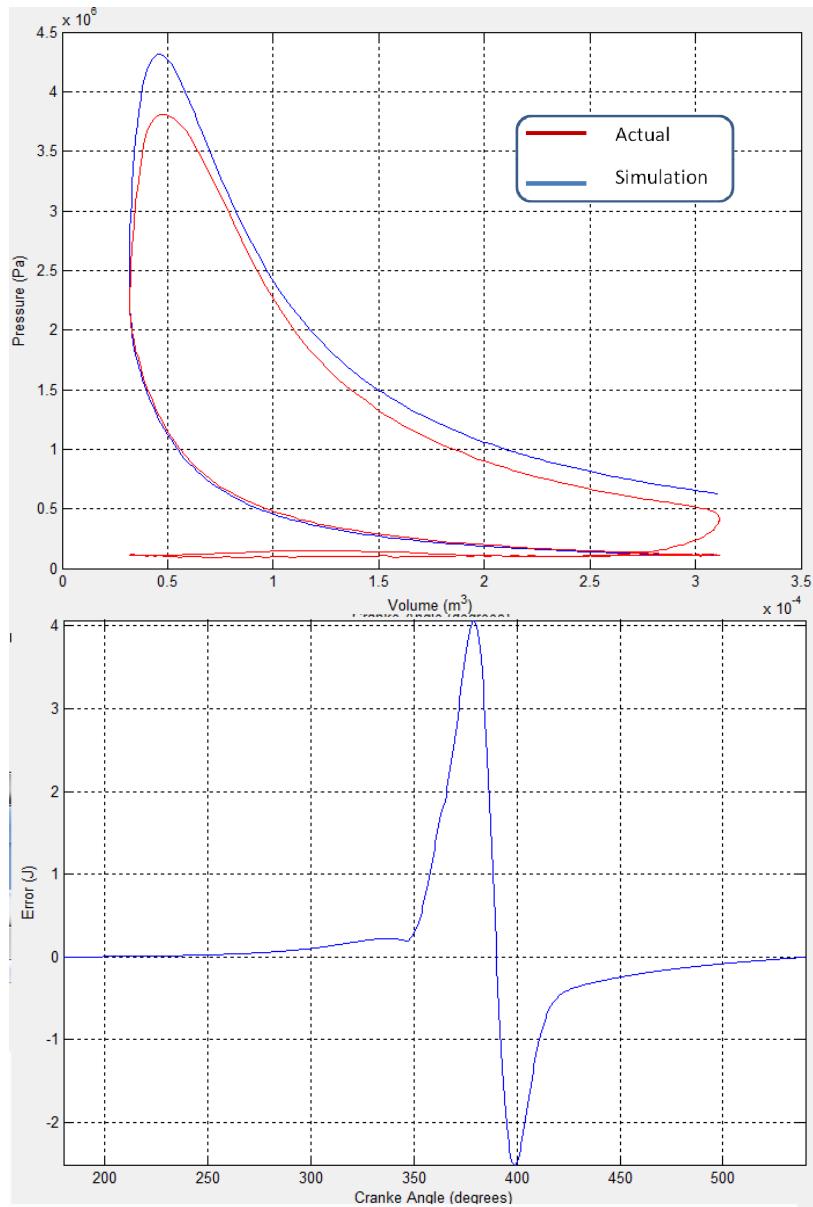


**Figure 25 - Error of Constant Specific Heat**

Plotting error against CA (as shown in Figure 25) reveals that the error turns towards negative during compression, and back towards positive during combustion BTDC, cancelling each other's effect somewhat.

However the author did not agree with the constant specific heats assumption, in particular for the expansion strokes, since the composition is changing and thus so is its properties. Ackerman, M. (2009) did mention some limited success with this method. However the author was confident from the literature survey, that the limitation is not the method, but the implementation.

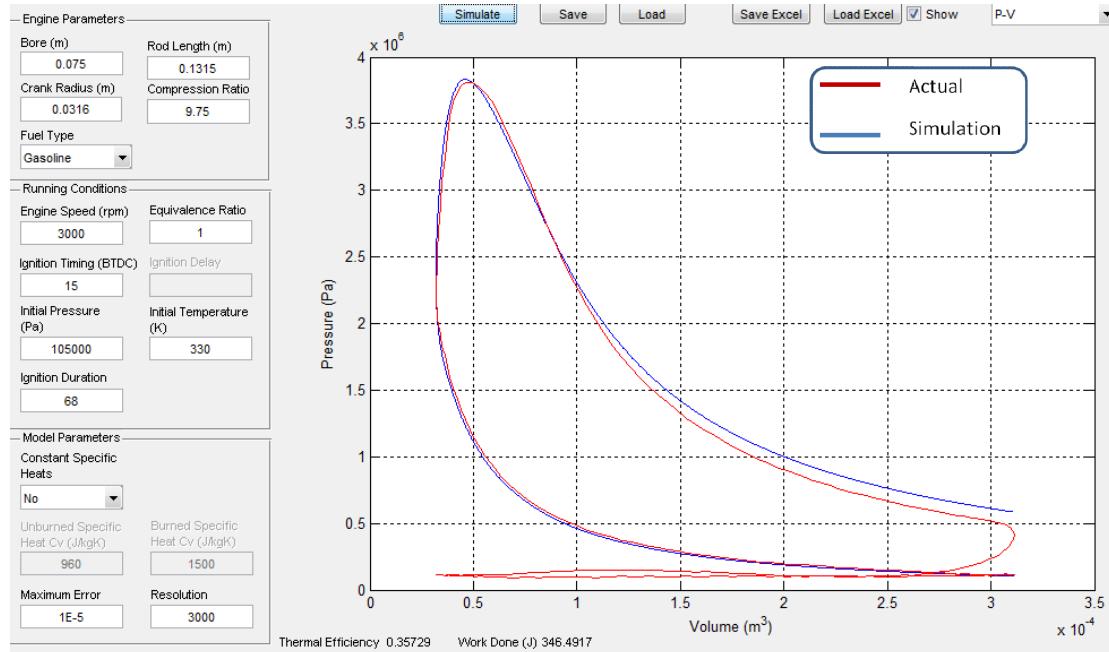
Upon running a simulation with variable specific heats as a function of temperature, the following was achieved:



**Figure 26 - High Error Threshold Simulation**

The indicator diagram reveals virtually no difference, however looking at the error plot reveals that the maximum error has increased by a multiple of 100. The error is only really increasing towards positive during the compression combustion BTDC. This was believed to be due to the fact, that an accurate temperature value is important to determine the

thermodynamic properties of that same step for which the temperature is being established. The simulation was re-run with a maximum preferred error of 1E-5. This produced the following:



**Figure 27 - Simulation Comparison**

It can be seen from Figure 27 that the varying specific heat method with a sufficient number of iterations of the Newton-Raphson method, has produced an indicator diagram that is so far the closest to the original data, while still retaining the high combustion efficiency expected to be present for IC engines.

It is now believed that the NASA polynomials failed in Ackerman, M., spreadsheet model, due to the cross dependency on an accurate temperature value, for which no iterative method was implemented. Having said so, doing this sort of simulation on a spreadsheet may be daunting. The choice to opt for an engineering scripting environment such as Matlab is showing itself to have been the better choice.

The simulation's results with the Newton-Raphson method applied were very promising and provided better matching peak pressures, and also the timing of the peak pressure is very similar. The net work done was still slightly higher (346J) than that calculated off the real data (314J), but was expected with the exclusion of the gas exchange process and thus neglecting the minor pumping losses as well (even at 100% throttle).

The thermal efficiency was simulated to be 36% while Ackerman, M., quotes 40%. However the author is of the opinion that 40% is slightly optimistic, and seems high due to the underestimation of the combustion efficiency. The author's own 36% efficiency is likely to be slightly too high since the actual net work is overestimated without the gas exchange.

Ironically the author could not find any other set of condition parameters that produce better results than those expected from the known running conditions and a combustion/ignition duration of 68CA.

## 6.2 CI Simulation

### Test Data Conditions

<b>Engine:</b>	2232cc diesel
<b>Ignition timing:</b>	2CA BTDC
<b>Equivalence Ratio</b>	~0.3-0.4
<b>Engine Speed:</b>	800rpm
<b>Fuel</b>	Pump fuel
<b>Ignition Timing</b>	

### Final Simulation Parameters

<b>Initial Temperature</b>	330 K
<b>Initial Pressure</b>	1.05bar
<b>Ignition timing:</b>	2CA BTDC
<b>Engine Speed:</b>	800rpm
<b>Fuel</b>	Diesel
<b>Equivalence Ratio</b>	0.38
<b>Ignition Duration</b>	120CA
<b>Ignition Delay</b>	2.8ms

The choice of parameters for the CI had to be chosen more intuitively. A 120CA combustion/ignition duration was chosen based on the suggestions of Heywood, John B. (1988). However the ignition delay was taken to be longer than the recommended 0.5-2ms due to the low speed / idle condition. Heywood, John B. (1988) does suggest that the ignition delay may be slower at low speeds and loads as discussed in section 2.6. Conveniently, the provider for the test data quoted the ignition timing as opposed to the injection timing. Presumably, they knew were likely to have estimated this value with sufficient accuracy through their engine management system and knowledge of their own chamber and injector design. Based on these parameters, the following result was achieved:

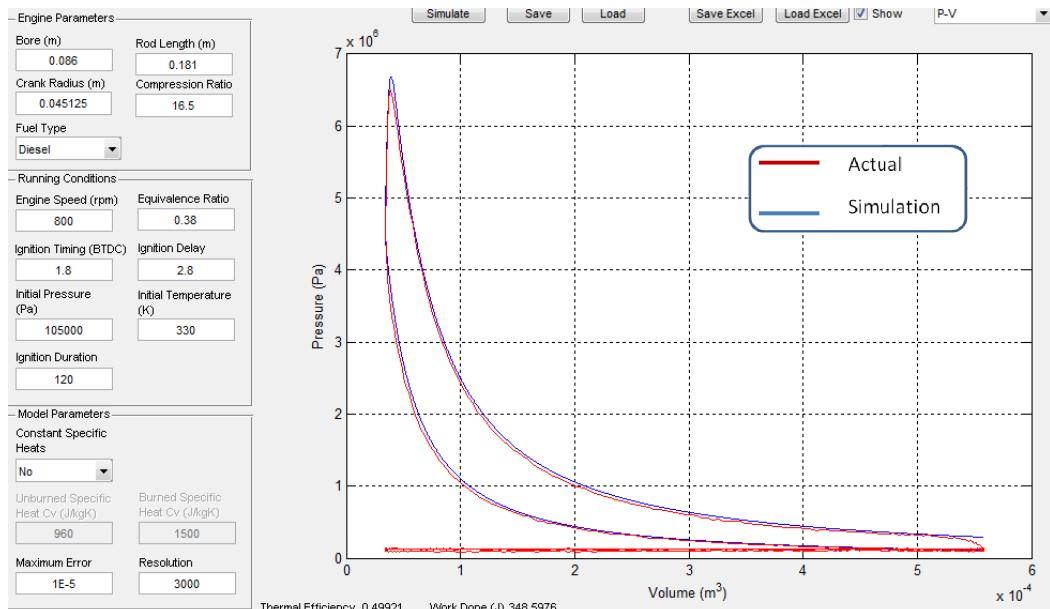
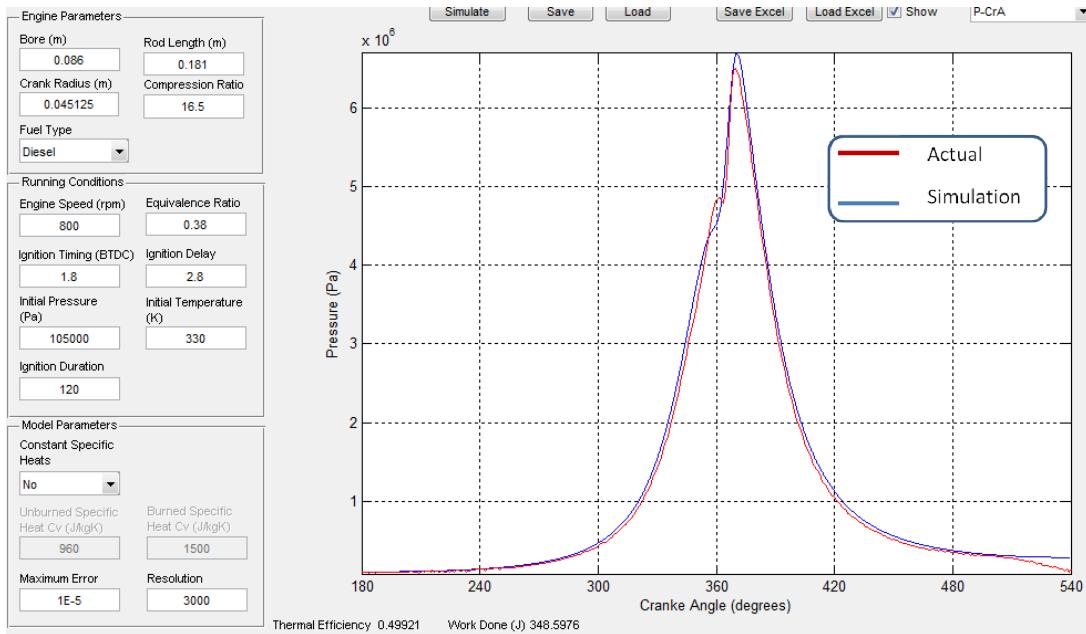


Figure 28 - CI Simulation Comparison P-V

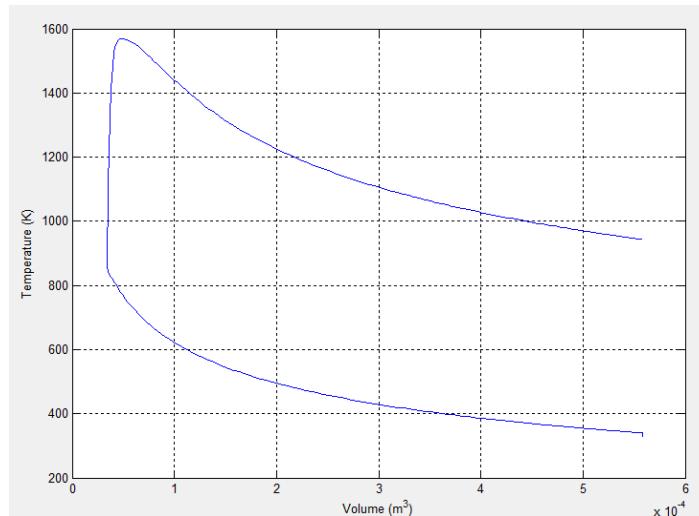


**Figure 29 - CI Simulation Comparison P-CA**

Figure 28 shows a very well matched p-V diagram, and even when considering Figure 29 which exposes the fine detail of transition from rapid burning to diffusion burning. The timing of transition is virtually identical, and thus so is the trend of the pressure rise.

Considering the greater number of degrees of freedom in simulation parameters for the combustion model for CI (entered from the GUI as well as the hard coded empirical constants), the results were very encouraging.

The simulation thermal efficiency was of about 50%. This is also believed to be slightly too high (though no comparison value is available). When considering CI engines, often pumping losses are dismissed due to the throttles operation. Nevertheless some pumping loss should exist, and is possibly more significant than that of the SI simulation at 100% throttle; since the swept volume is now larger (those give a greater area under the p-V diagram).



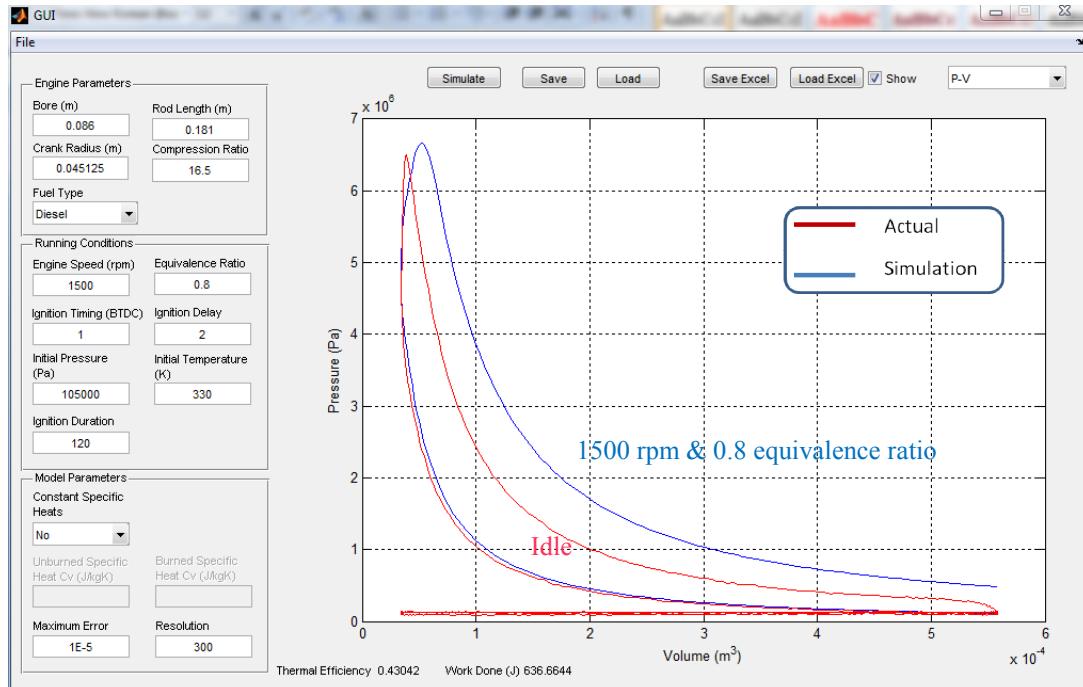
**Figure 30 - Temperature Range**

Plotting a temperature-volume graph also reveals that the peak temperatures are of around 1600K, within the area of operation where the estimated gas composition from the water-gas equilibrium was a fair assumption even for such a CI engine simulation.

### 6.3 Final Conclusions

From the completion of this Engine Sim tool set, it was exciting to virtually experience in person via the simulation, the tremendous advantage of running such high compression ratios. The standard Diesel cycle analysis originally indicated that CI engine should be of a lower thermal efficiency than that of a SI engine based on the thermal efficiency equation for the standard cycles.

Using the Engine Sim tool to try and predict the behaviour at higher loads and speeds was now possible (at least from a qualitative perspective). An increase in load and speed would cause the fuel-air mix to be richer then at idle, ignition delay to be less and possibly an earlier injection. Such conditions gave the following result:



**Figure 31 - Comparison of different speed and loads for CI**

This is a clear instance of where the developed tools were useful to run ‘what if’ scenarios. The result is very similar to that expected from understanding of the standard Diesel cycle. The increase in work done is achieved by extended the high pressure period similar to a similar effect of that cut-off ratio. This extra work output is at the cost of a reduction in thermal efficiency from 50% to 43% (based on the simulation). This is in line with the theory of the standard Diesel cycle.

The author is content with the overall results and believes that the original goals have been met, while also creating an awareness of several areas that may be expanded further.

## **7. Further Work**

This work proved successful, and as with all constructive research work, it is bound to prompt for further investigation in areas originally omitted or not considered of relevance at the time. Such areas are:

- Including Gas Exchange Models – Currently the model is useful but incomplete to truly simulate a full cycle. Including the gas exchange would complete the real physical loop. It would also permit more objective efficiency values to be calculated as well as helping demonstrate the key difference in engine governing mechanisms of CI and SI engines.
- Including Exhaust Gas Recirculation EGR and Residual Gas – Currently the model assumes only fresh air to occupy the cylinder. In actual fact, some residual gas may remain or intentional residual gas is contained through methods such as negative valve overlap, or external exhaust gas recirculation. The composition models can handle pre-existing residual exhaust gases, and therefore to accomplish this addition, one would have to carefully re-link the sub models together with a gas exchange gas model.
- Further Real Test Data Comparison – So far the data collected and compared with proved useful; however several uncertainties remain in the available data to fully constrain the conditions of the simulation. Fully constraining these parameters would help further understand the current model's limitations and/or help calibrate any empirical constants used.
- Heat Loss – During an engine cycle, it is a fact that the oil and coolant warm up. So much so that these is a critical detail in component design. Engine management systems vary ignition timing and fuel-air ratios to control how rapidly or not the engine warms up. This all indicates to a degree of heat transfer through the cylinder wall.

Certainly, the developed tools discussed in this work, provide a solid platform to tackle the areas mentioned above for further work.

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- STONE, RICHARD, 1999. *Introduction to Internal Combustion Engines, 3<sup>rd</sup> edition*. Macmillan Press Ltd.
- TURNS, STEPHEN R., 2000. *An Introduction to Combustion 2<sup>nd</sup> edition*. McGraw Hill.
- WATSON N. PILLEY A. D. and MARZOUK M., 1980. *A Combustion Correlation for Diesel Engine Simulation*. SAE Paper 760128.

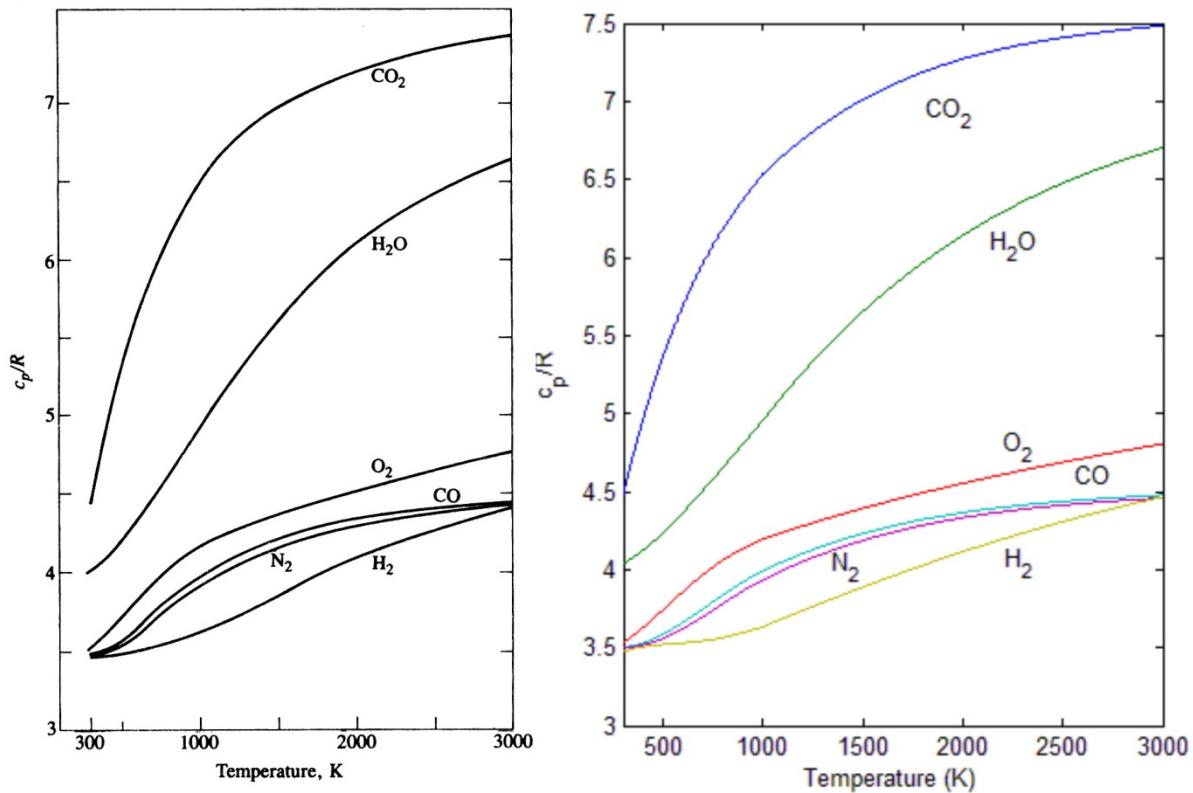
## Appendix A – Function List

Function Name	Output = Function ( Input(s) )
<b>BComposition</b>	[ Burned mole fraction array ] = BComposition( Equiv, NOr, HCr, T )
<b>BModel</b>	[ xb ] = BModel( duartion, CrA, ign, Ne, fueltype [equiv] [ign_delay_ms] )
<b>CEfficiency</b>	[ efficiency ] = CEfficiency( fueltype, equiv )
<b>CProperties</b>	[ Cv, molarM, R ] = CProperties( T, species )
<b>CrV</b>	[ V ] = CrV( Angle, Vc, CR, Ratio_RC )
<b>ESim</b>	[ P, T, V, CrA, xb ] = ESim( B, I, a, CR, PInit, TInit, motoring, res, accuracy, [optional parameters] )
<b>GRelations</b>	[ L Ratio_RC PA Vs Vc ] = GRelations( B, I, a, CR )
<b>GUI</b>	Launches GUI interface
<b>HCr</b>	[ HC_ratio ] = HCr( fueltype )
<b>HFuel</b>	[ h ] = HFuel( fueltype )
<b>MProperties</b>	[ Cv M R ] =MProperties ( T, component, component ratio, ... )
<b>TCombustion</b>	[ dT ] = TCombustion( mode, mf, mc, xb1, xb2, h, Cv, [options] )
<b>TCompression</b>	[ T_i+1 ] = TCompression( mode=1, T_i, P_i, V_i, V_i+1, mc, Cv, [optional parameters] )
<b>UComposition</b>	[ Unburned Mole Fraction Array ] = UComposition( EquivilanceRatio, NOr, HCr, T, Mf, xb )
<b>WDone</b>	[ Work ] = WDone( P, V )

**Table 7 - Function List**

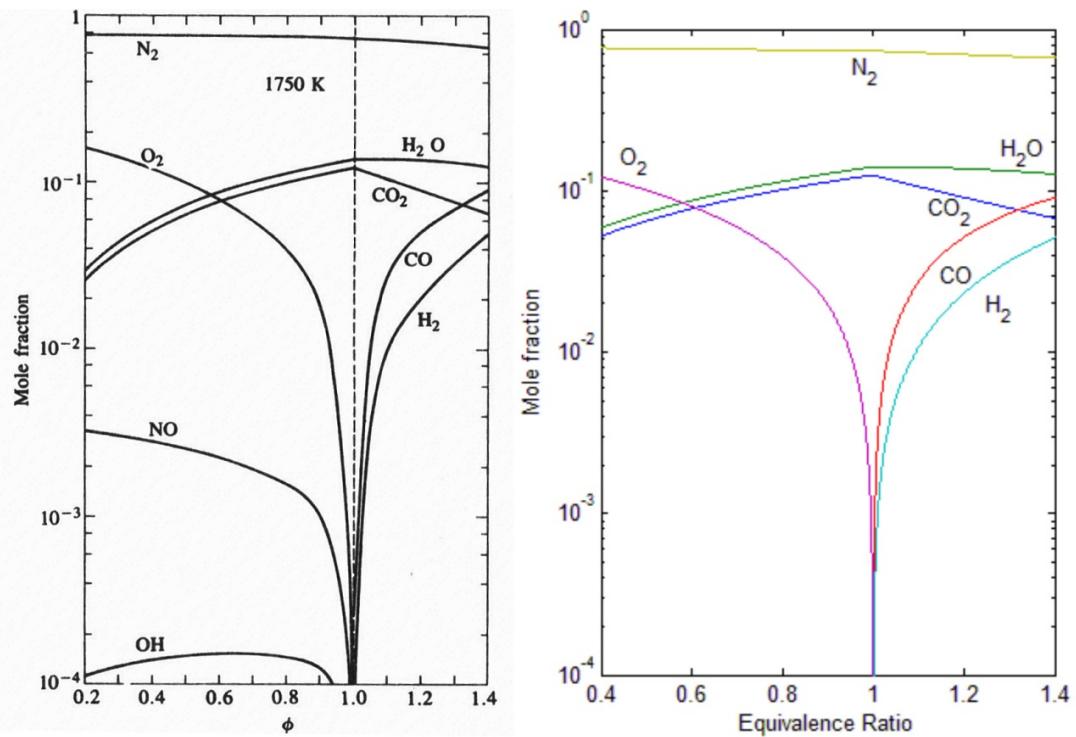
Each function contains its own help command in Matlab for further syntax help and example usage.

## Appendix B – Validation Functions



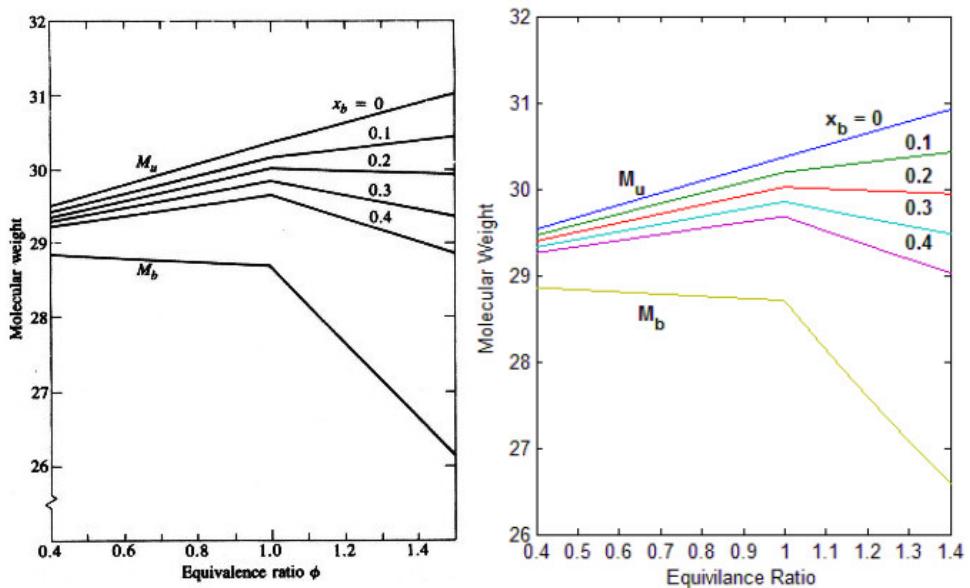
**Figure 32 - Comparison between Cp properties (Left: Heywood John .B., 1988; Right: Author)**

Figure 32 demonstrates that **CProperties(...)** functions well, as it has calculated the specific heat at constant pressure in agreement with Heywood B. John (1988)



**Figure 33 - Comparison between Exhaust Composition for Full Equilibrium and Water-Gas Shift (Left: Heywood John .B., 1988; Right: Author)**

Figure 33 demonstrates that water-gas shifts is sufficient to calculate the major species of the exhaust gas composition at low temperatures (below 1500-2000K). This also demonstrates that the function **BComposition(...)** is an adequate model for the water-gas shift approximation.



**Figure 34 - Molecular Weight Variation with Fraction Burn and Equivalence Ratio (Left: Heywood John .B., 1988; Right: Author)**

Figure 34 demonstrates that the **MProperties(...)**, **UComposition(...)** and **BComposition(...)** functions are calculating the correct composition and thus the correct molecular weights to establish the mixture's molecular weight.

## Appendix C – Code Listing

The main code has been listed here. The code for the GUI is omitted here but included in the accompanying CD.

```
function [ B ] = BComposition( Equiv, NOr, HCr, T )
%   [ Burned mole fraction array ] = BComposition( Equiv, NOr, HCr, T )
% Where [ ... ] = [0 nO2 nN2 nCO2 nH2O nCO nH2];
%
% Inputs:
% Equiv : Equivilance ratio for which the composition is calculated.
% NOr   : Nitrogen to Oxygen ratio (usually 3.77)
% HCr   : Hydrogen to Carbon ratio of fuel
% T     : Temperature at which process is calculated (approximate <1700K)

eta = 4 / (4 + HCr);

if Equiv <= 1
    nCO2 = eta * Equiv;
    nH2O = 2*(1-eta)*Equiv;
    nCO = 0;
    nH2 = 0;
    nO2 = 1 - Equiv;
    nN2 = NOr;
else
    K = exp(2.743 - 1.761E3/T - 1.611E6/T^2 + 0.2803E9/T^3);
    a = (K-1);
    b = -(K*(2*(Equiv - 1) + eta*Equiv) + 2*(1-eta*Equiv));
    c = 2*K*eta*Equiv*(Equiv-1);
    z = (-b-sqrt(b^2-4*a*c))/(2*a);

    nCO2 = eta * Equiv - z;
    nH2O = 2*(1-eta*Equiv) + z;
    nCO = z;
    nH2 = 2*(Equiv-1) - z;
    nO2 = 0;
    nN2 = NOr;
end
B = [0 nO2 nN2 nCO2 nH2O nCO nH2];
B = B ./ sum(B);

end
```

---

```
function [ xb ] = BModel( duration, CrA, ign, Ne, fueltype, varargin )
%   [ xb ] = BModel( duartion, CrA, ign, Ne, fueltype [equiv]
[ign_delay_ms] )
%
%   equiv and ign_delay_ms needed if fuel type is diesel.
%
%   BModel calculates the fraction burn. The model used depends on the fuel
%   type, for diesel, a diesel burning model. For other fuel types, the
%   generic gasoline model is used.
%
%   Diesel additional inputs: equivalence ratio, and ignition delay

if strcmp(fueltype, 'diesel') == 1
```

```

numvarargs = size(varargin, 2);
if numvarargs ~= 2
    error('equivalence ratio needed for diesel combustion model and
ignition delay');
end
equiv = varargin{1};
ign_delay_ms = varargin{2};

a = 0.8;
% 0.8 < a < 0.95
b = 0.45;
% 0.25 < b < 0.45
c = 0.25;
% 0.25 < c < 0.5

beta = 1 - (a*equiv^b)/(ign_delay_ms^c);
temp = CrA - (360-ign);
if temp < 0;
    xb = 0;
elseif ((temp >= 0) && (temp < duration))
    K1 = 2 + 1.25 * (10^-8)*(ign_delay_ms * Ne)^2.4;
    K2 = 5000;
    K3 = 14.2/(equiv^0.644);
    K4 = 0.79*K3^0.25;
    tdash = temp/duration;
    f2 = 1 - exp(-K3*tdash^K4);
    f1 = 1 - (1 - tdash^K1)^K2;
    xb = beta*f1 + (1 - beta)*f2;
else
    xb = 1;
end
else
    temp = CrA - (360-ign);
    if temp < 0;
        xb = 0;

    elseif ((0 <= temp))
        a = 5;
        m = 2;
        xb = 1 - exp(-a*((temp)/duration)^(m+1));
    else
        xb = 1;
    end
end
end

```

---

```

function [ Cv, M, R ] = CProperties( T, species )
% [ Cv, molarM, R ] = CProperties( T, species )
%
% Can evaluate properties of:
% CO2, H2O, N2, O2, CO, H2, H, O, OH, NO
% and
% gasoline, diesel, isoctane, propane

% Data taken and adapted from
% David R. Buttsworth, 2002, "Spark Ignition Internal Combustion Engine
% Modelling using Matlab", who took the data from:
% 1. Ferguson C.R., 1986, "Internal Combustion Engines", Wiley;

```

```

% 2. Heywood J.B., 1988, "Internal Combustion Engine Fundamentals",
%     McGraw-Hill;
% 3. Raine R. R., 2000, "ISIS_319 User Manual", Oxford Engine Group.

ACO2l= [0.24007797E+01 0.87350957E-02 -0.66070878E-05 0.20021861E-08
0.63274039E-15 -0.48377527E+05 0.96951457E+01];
AH20l= [0.40701275E+01 -0.11084499E-02 0.41521180E-05 -0.29637404E-08
0.80702103E-12 -0.30279722E+05 -0.32270046E+00];
AN2l = [0.36748261E+01 -0.12081500E-02 0.23240102E-05 -0.63217559E-09 -
0.22577253E-12 -0.10611588E+04 0.23580424E+0];
AO2l = [0.36255985E+01 -0.18782184E-02 0.70554544E-05 -0.67635137E-08
0.21555993E-11 -0.10475226E+04 0.43052778E+01];
AC0l = [0.37100928E+01 -0.16190964E-02 0.36923594E-05 -0.20319674E-08
0.23953344E-12 -0.14356310E+05 0.29555350E+01];
AH2l = [0.30574451E+01 0.26765200E-02 -0.58099162E-05 0.55210391E-08 -
0.18122739E-11 -0.98890474E+03 -0.22997056E+01];
AHl = [0.25000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.25471627E+05 -0.46011762E+00];
AO1 = [0.29464287E+01 -0.16381665E-02 0.24210316E-05 -0.16028432E-08
0.38906964E-12 0.29147644E+05 0.29639949E+01];
AOHl = [0.38375943E+01 -0.10778858E-02 0.96830378E-06 0.18713972E-09 -
0.22571094E-12 0.36412823E+04 0.49370009E+00];
ANO1 = [0.40459521E+01 -0.34181783E-02 0.79819190E-05 -0.61139316E-08
0.15919076E-11 0.97453934E+04 0.29974988E+01];

ACO2h= [0.44608041E+01 0.30981719E-02 -0.12392571E-05 0.22741325E-09 -
0.15525954E-13 -0.48961442E+05 -0.98635982E+00];
AH2Oh= [0.27167633E+01 0.29451374E-02 -0.80224374E-06 0.10226682E-09 -
0.48472145E-14 -0.29905826E+05 0.66305671E+01];
AN2h = [0.28963194E+01 0.15154866E-02 -0.57235277E-06 0.99807393E-10 -
0.65223555E-14 -0.90586184E+03 0.61615148E+01];
AO2h = [0.36219535E+01 0.73618264E-03 -0.19652228E-06 0.36201558E-10 -
0.28945627E-14 -0.12019825E+04 0.36150960E+01];
ACOh = [0.29840696E+01 0.14891390E-02 -0.57899684E-06 0.10364577E-09 -
0.69353550E-14 -0.14245228E+05 0.63479156E+01];
AH2h = [0.31001901E+01 0.51119464E-03 0.52644210E-07 -0.34909973E-10
0.36945345E-14 -0.87738042E+03 -0.19629421E+01];
Ahh = [0.25000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.25471627E+05 -0.46011763E+00];
AOh = [0.25420596E+01 -0.27550619E-04 -0.31028033E-08 0.45510674E-11 -
0.43680515E-15 0.29230803E+05 0.49203080E+01];
AOHh = [0.29106427E+01 0.95931650E-03 -0.19441702E-06 0.13756646E-10
0.14224542E-15 0.39353815E+04 0.54423445E+01];
ANOh = [0.31890000E+01 0.13382281E-02 -0.52899318E-06 0.95919332E-10 -
0.64847932E-14 0.98283290E+04 0.67458126E+01];

Adiesel      = [-9.1063 246.97 -143.74 32.329 0.0518 -50.128];
Agasoline    = [-24.078 256.63 -201.68 64.750 0.5808 -27.562];
Aisooctane   = [-0.55313 181.62 -97.787 20.402 -0.03095 -60.751];
Apropane     = [-1.4867 74.339 -39.065 8.0543 0.01219 -27.313];

if strcmp(species, 'diesel') == 1
    A = Adiesel;
    T = T/1000;
    molM = 148.6;
    R = 8314.5/molM;
    Cp = sum(A*[1 T T^2 T^3 T^-2 0])*4187/molM;
elseif strcmp(species, 'gasoline') == 1
    A = Agasoline;

```

```

T = T/1000;
molM = 114.8;
R = 8314.5/molM;
Cp = sum(A*[1 T T^2 T^3 T^-2 0])*4187/molM;
elseif strcmp(species, 'isoctane') == 1
A = Isooctane;
T = T/1000;
molM = 114.2;
R = 8314.5/molM;
Cp = sum(A*[1 T T^2 T^3 T^-2 0])*4187/molM;
elseif strcmp(species, 'propane') == 1
A = Apropane;
T = T/1000;
molM = 44.1;
R = 8314.5/molM;
Cp = sum(A*[1 T T^2 T^3 T^-2 0])*4187/molM;
else
if T < 1000
switch species
case 'CO2'
A = ACCO2l;
molM = 44;
case 'H2O'
A = AH2Ol;
molM = 18;
case 'N2'
A = AN2l;
molM = 28.16; %atmospheric Nitrogen;
case 'O2'
A = AO2l;
molM = 32;
case 'CO'
A = ACOL;
molM = 28;
case 'H2'
A = AH2l;
molM = 2;
case 'H'
A = AHL;
molM = 1;
case 'O'
A = AOL;
molM = 16;
case 'OH'
A = AOHL;
molM = 17;
case 'NO'
A = ANOL;
molM = 44.16;
end
else
switch species
case 'CO2'
A = ACCO2h;
molM = 44;
case 'H2O'
A = AH2Oh;
molM = 18;
case 'N2'
A = AN2h;
molM = 28.16; %atmospheric Nitrogen;

```

```

        case 'O2'
            A = AO2h;
            molM = 32;
        case 'CO'
            A = ACOh;
            molM = 28;
        case 'H2'
            A = AH2h;
            molM = 2;
        case 'H'
            A = AHh;
            molM = 1;
        case 'O'
            A = AOh;
            molM = 16;
        case 'OH'
            A = AOOh;
            molM = 17;
        case 'NO'
            A = ANOh;
            molM = 44.16;
        end
    end
    R = 8314.5/molM; % kJ / kmolK
    Cp = sum(A*[1 T T^2 T^3 T^4 0 0])*R; % J / kgK
end
M = molM;
Cv = Cp - R; % kJ / kgK
end

```

---

```

function [ V ] = CrV( CrA, Vc, CR, Ratio_RC )
% [ V ] = CrV( Angle, Vc, CR, Ratio_RC )
% Returns the cylinder volume for a given:
% CrA : Crank Angle in degrees
% Vc : Clearane Volume
% CR : Compression Ratio
% Ratio_RC: Ratio of Connectin Rod to crank radius

V = Vc * (1 + 0.5.* (CR - 1).* (Ratio_RC + 1 - cosd(CrA) - sqrt(Ratio_RC.^2
- (sind(CrA)).^2)));
end

```

---

```

function [ P T V CrA xb nTH Error ] = ESim( B, l, a, CR, PInit, TInit,
motoring, res, accuracy, varargin )
% [ P, T, V, CrA, xb ] = ESim( B, l, a, CR, PInit, TInit, motoring, res,
accuracy, [optional parameters] )
% [] = ESim( B, l, a, CR, PInit, TInit, motoring, res, accuracy )
% [] = ESim( B, l, a, CR, PInit, TInit, motoring, res, accuracy, N (rpm),
equiv, duration, ign, fueltype=gasoline/isooctane/propane, property_type=2
)
% [] = ESim( B, l, a, CR, PInit, TInit, motoring, res, accuracy, N (rpm),
equiv, duration, ign, fueltype=gasoline/isooctane/propane, property_type=1,
Cv_u, Cv_b )
% [] = ESim( B, l, a, CR, PInit, TInit, motoring, res, accuracy, N (rpm),
equiv, duration, ign, fueltype=diesel, ignition delay, property_type=2)
% [] = ESim( B, l, a, CR, PInit, TInit, motoring, res, accuracy, N (rpm),
equiv, duration, ign, fueltype=diesel, ignition delay, property_type=1,
Cv_u, Cv_b )

```

```

% Outputs
% P:      Pressure
% T:      Temperature
% V:      Volume
% CrA:    Crank Angle
% xb:     Fraction burn
% Error:  Error measure of approximation

step = 360/res; % number of steps for a complete revolution
%step is used to pre-assign variables and/or maximum loop counters

NOr = 3.773; %Heywood

CrA(res) = 0;
V(res) = 0;
xb(res) = 0;
T(res) = 0;
P(res) = 0;
Error(res) = 0;

[ Ratio_RC Vc ] = GRelations( B, l, a, CR);

if motoring == 1
    flag = 0;
else
    equiv = varargin{1};
    N = varargin{2};
    duration = varargin{3};
    ign = varargin{4};
    fueltype = varargin{5};

    if strcmp(fueltype, 'diesel') == 1
        flag = 1;
    elseif strcmp(fueltype, 'gasoline') == 1
        flag = 2;
    elseif strcmp(fueltype, 'isoctane') == 1
        flag = 3;
    elseif strcmp(fueltype, 'propane') == 1
        flag = 4;
    end
    h = HFuel(fueltype);
    Efficiency = CEfficiency(fueltype, equiv);
end
if flag == 1
    ign_delay_ms = varargin{6};
    propertytype = varargin{7};
    if propertytype == 1
        Cv_u = varargin{8};
        Cv_b = varargin{9};
    else
        Cv_mix(res)=0;
        Cv_air(res) = 0;
    end
elseif flag > 1
    propertytype = varargin{6};
    if propertytype == 1
        Cv_u = varargin{7};
        Cv_b = varargin{8};
    end

```

```

Cv_mix(res)=0;
Cv_air(res) = 0;
end

for cnt=1:res
CrA(cnt)= (cnt*step-step)+180;
V(cnt) = CrV(CrA(cnt), Vc, CR, Ratio_RC);

if cnt == 1
    T(cnt) = TInit;
    P(cnt) = PInit;
    [ Cv_air(cnt), M_air R_air ] = MProperties(T(cnt), 'O2', 1, 'N2',
NOr);
    mc = P(cnt)*V(cnt)/(R_air*T(cnt));
    xb(cnt) = 0;
    if flag ~= 0
        [ ~, M_fuel, ~ ] = CProperties(T(cnt), fueltype);
        [MoleFr] = UComposition(equiv, NOr, HCr(fueltype), T(cnt),
M_fuel, 0);
        [ Cv_mix , ~, ~ ] = MProperties(T(cnt), fueltype, MoleFr(1),
'O2', MoleFr(2), 'N2', MoleFr(3), 'CO2', MoleFr(4), 'H2O', MoleFr(5),
'CO', MoleFr(6), 'H2', MoleFr(7));
        n_air = mc / M_air; % number of moles of air in cylinder
        n_fuel = MoleFr(1) * n_air / ( 1 - MoleFr(1)); % number of
moles of fuel
        mfuel = n_fuel * M_fuel;
    else
        mfuel = 0;
    end

else
    if flag == 0
        % Motoring
        xb(cnt) = 0;
        nTH = 0;
        [% Cv_air(cnt) , ~, R_air ] = MProperties(T(cnt), 'O2', 1,
'N2', NOr);
        Cv_air(cnt) = 723.5325;
        T(cnt) = TCompression( 2, T(cnt-1), P(cnt-1), V(cnt-1), V(cnt),
mc, Cv_air(cnt));
        P(cnt) = P(cnt-1)* V(cnt-1)*T(cnt)/(V(cnt)*T(cnt-1));
        Error(cnt) = mc*Cv_air(cnt)*T(cnt)- mc*Cv_air(cnt-1)*T(cnt-1) +
0.5*(P(cnt)+P(cnt-1))*(V(cnt)-V(cnt-1));
        cycle_count = 0;
        while (((Error(cnt) > accuracy) || (Error(cnt) < -1*accuracy))
&& (cycle_count < 200))
            cycle_count = cycle_count + 1;
            T(cnt) = T(cnt) - Error(cnt)/(mc*Cv_air(cnt));
            P(cnt) = P(cnt-1) * V(cnt-1)*T(cnt)/(V(cnt)*T(cnt-1));
            [% Cv_air(cnt) , ~, R_air ] = MProperties(T(cnt), 'O2', 1,
'N2', NOr);
            Cv_air(cnt) = 723.5325;
            Error(cnt) = mc*Cv_air(cnt)*T(cnt)- mc*Cv_air(cnt-1)*T(cnt-1) +
0.5*(P(cnt)+P(cnt-1))*(V(cnt)-V(cnt-1));
        end
    elseif flag == 1
        % Diesel - No fuel in compression

```

```

        xb(cnt) = Efficiency * BModel( duration, CrA(cnt), ign, N,
fueltype, equiv, ign_delay_ms );
        [MoleFr] = UComposition(equiv, NOr, HCr(fueltype), T(cnt),
M_fuel, xb(cnt));

        if propertytype == 2
            [ Cv_mix(cnt) , ~, ~ ] = MProperties(T(cnt-1), fueltype, 0,
'02', MoleFr(2), 'N2', MoleFr(3), 'CO2', MoleFr(4), 'H2O', MoleFr(5), 'CO',
MoleFr(6), 'H2', MoleFr(7));
            T(cnt) = TCompression(propertytype, T(cnt-1), P(cnt-1),
V(cnt-1), V(cnt), mc, Cv_mix(cnt));
            T_comb = TCombustion(propertytype, mfuel, mc, xb(cnt-1),
xb(cnt), h, Cv_mix(cnt));
            T(cnt) = T(cnt) + T_comb;
            P(cnt) = P(cnt-1)* V(cnt-1)*T(cnt)/(V(cnt)*T(cnt-1));
            Error(cnt) = mc*Cv_mix(cnt)*T(cnt)- mc*Cv_mix(cnt-1)*T(cnt-
1) + 0.5*(P(cnt)+P(cnt-1))*(V(cnt)-V(cnt-1)) - T_comb*mc*Cv_mix(cnt-1);
            cycle_count = 0;
            while (((Error(cnt) > accuracy) || (Error(cnt) < -
1*accuracy)) && (cycle_count < 200))
                cycle_count = cycle_count + 1;
                T(cnt) = T(cnt) - Error(cnt)/(mc*Cv_mix(cnt));
                P(cnt) = P(cnt-1) * V(cnt-1)*T(cnt)/(V(cnt)*T(cnt-1));
                [MoleFr] = UComposition(equiv, NOr, HCr(fueltype),
T(cnt), M_fuel, xb(cnt));
                [ Cv_mix(cnt) , ~, ~ ] = MProperties(T(cnt-1),
fueltype, 0, '02', MoleFr(2), 'N2', MoleFr(3), 'CO2', MoleFr(4), 'H2O',
MoleFr(5), 'CO', MoleFr(6), 'H2', MoleFr(7));
                Error(cnt) = mc*Cv_mix(cnt)*T(cnt)- mc*Cv_mix(cnt-
1)*T(cnt-1) + 0.5*(P(cnt)+P(cnt-1))*(V(cnt)-V(cnt-1)) -
T_comb*mc*Cv_mix(cnt-1);
            end
        else
            T(cnt) = TCompression(propertytype, T(cnt-1), P(cnt-1),
V(cnt-1), V(cnt), mc, Cv_u, Cv_b, xb(cnt));
            T_comb = TCombustion(propertytype, mfuel, mc, xb(cnt-1),
xb(cnt), h, Cv_u, Cv_b);
            T(cnt) = T(cnt) + T_comb;
            P(cnt) = P(cnt-1)* V(cnt-1)*T(cnt)/(V(cnt)*T(cnt-1));
            Error(cnt) = mc*((1-xb(cnt))*Cv_u+xb(cnt)*Cv_b)*(T(cnt)-
T(cnt-1)) + 0.5*(P(cnt)+P(cnt-1))*(V(cnt)-V(cnt-1)) - T_comb*mc*((1-
xb(cnt))*Cv_u+xb(cnt)*Cv_b);
            cycle_count = 0;
            while (((Error(cnt) > accuracy) || (Error(cnt) < -
1*accuracy)) && (cycle_count < 200))
                cycle_count = cycle_count + 1;
                T(cnt) = T(cnt) - Error(cnt)/(mc*((1-
xb(cnt))*Cv_u+xb(cnt)*Cv_b));
                P(cnt) = P(cnt-1) * V(cnt-1)*T(cnt)/(V(cnt)*T(cnt-1));
                Error(cnt) = mc*((1-
xb(cnt))*Cv_u+xb(cnt)*Cv_b)*(T(cnt)- T(cnt-1)) + 0.5*(P(cnt)+P(cnt-
1))*(V(cnt)-V(cnt-1)) - T_comb*mc*((1-xb(cnt))*Cv_u+xb(cnt)*Cv_b);
            end
        end
    elseif ( (flag > 1) && (flag <=4) )
        % Gasoline / Isooctane / Propane
        xb(cnt) = Efficiency * BModel( duration, CrA(cnt), ign, N,
fueltype );
        [MoleFr] = UComposition(equiv, NOr, HCr(fueltype), T(cnt-1),
M_fuel, xb(cnt));

```

```

        if propertytype == 2
            [ Cv_mix(cnt) , ~, ~ ] = MProperties(T(cnt-1), fueltype,
MoleFr(1), 'O2', MoleFr(2), 'N2', MoleFr(3), 'CO2', MoleFr(4), 'H2O',
MoleFr(5), 'CO', MoleFr(6), 'H2', MoleFr(7));
            T(cnt) = TCompression(propertytype, T(cnt-1), P(cnt-1),
V(cnt-1), V(cnt), mc, Cv_mix(cnt));
            T_comb = TCombustion(propertytype, mfuel, mc, xb(cnt-1),
xb(cnt), h, Cv_mix(cnt));
            T(cnt) = T(cnt) + T_comb;
            P(cnt) = P(cnt-1)* V(cnt-1)*T(cnt)/(V(cnt)*T(cnt-1));
            Error(cnt) = mc*Cv_mix(cnt)*T(cnt)- mc*Cv_mix(cnt-1)*T(cnt-
1) + 0.5*(P(cnt)+P(cnt-1))*(V(cnt)-V(cnt-1)) - T_comb*mc*Cv_mix(cnt-1);
            cycle_count = 0;
            while (((Error(cnt) > accuracy) || (Error(cnt) < -
1*accuracy)) && (cycle_count < 200))
                cycle_count = cycle_count + 1;
                T(cnt) = T(cnt) - Error(cnt)/(mc*Cv_mix(cnt));
                P(cnt) = P(cnt-1) * V(cnt-1)*T(cnt)/(V(cnt)*T(cnt-1));
                [MoleFr] = UComposition(equiv, NOr, HCr(fueltype),
T(cnt), M_fuel, xb(cnt));
                [ Cv_mix(cnt) , ~, ~ ] = MProperties(T(cnt-1),
fueltype, MoleFr(1), 'O2', MoleFr(2), 'N2', MoleFr(3), 'CO2', MoleFr(4),
'H2O', MoleFr(5), 'CO', MoleFr(6), 'H2', MoleFr(7));
                Error(cnt) = mc*Cv_mix(cnt)*T(cnt)- mc*Cv_mix(cnt-
1)*T(cnt-1) + 0.5*(P(cnt)+P(cnt-1))*(V(cnt)-V(cnt-1)) -
T_comb*mc*Cv_mix(cnt-1);
            end
        else
            T(cnt) = TCompression(propertytype, T(cnt-1), P(cnt-1),
V(cnt-1), V(cnt), mc, Cv_u, Cv_b, xb(cnt));
            T_comb = TCombustion(propertytype, mfuel, mc, xb(cnt-1),
xb(cnt), h, Cv_u, Cv_b);
            T(cnt) = T(cnt) + T_comb;
            P(cnt) = P(cnt-1)* V(cnt-1)*T(cnt)/(V(cnt)*T(cnt-1));
            %P(cnt) = mc*R_air*T(cnt)/V(cnt);
            Error(cnt) = mc*((1-xb(cnt))*Cv_u+xb(cnt)*Cv_b)*(T(cnt)-
T(cnt-1)) + 0.5*(P(cnt)+P(cnt-1))*(V(cnt)-V(cnt-1)) - T_comb*mc*((1-
xb(cnt))*Cv_u+xb(cnt)*Cv_b);
            cycle_count = 0;
            while (((Error(cnt) > accuracy) || (Error(cnt) < -
1*accuracy)) && (cycle_count < 200))
                cycle_count = cycle_count + 1;
                T(cnt) = T(cnt) - Error(cnt)/(mc*((1-
xb(cnt))*Cv_u+xb(cnt)*Cv_b));
                P(cnt) = P(cnt-1) * V(cnt-1)*T(cnt)/(V(cnt)*T(cnt-1));
                Error(cnt) = mc*((1-
xb(cnt))*Cv_u+xb(cnt)*Cv_b)*(T(cnt) - T(cnt-1)) + 0.5*(P(cnt)+P(cnt-
1))*(V(cnt)-V(cnt-1)) - T_comb*mc*((1-xb(cnt))*Cv_u+xb(cnt)*Cv_b);
            end
        end
    end
if flag > 0
    nTH = WDone(P,V) / (Efficiency*mfuel*h);
end
end

```

```

function [ Ratio_RC Vc ] = GRelations( B, l, a, CR )
%   [ L Ratio_RC PA Vs Vc ] = GRelations( B, l, a, CR )
%   Gives the stroke (L), ratio of con rod length to crank radius
% (Ratio_RC),
%   piston area (PA), swept volume and maximum volume (Vmax)

% As defined by Heywood J.B., 1988, "Internal Combustion Engine
% Fundamentals", McGraw-Hill;

L = 2 * a;
Ratio_RC = 1/a;
PA = pi*B^2/4;
Vs = L * PA;
Vc = Vs / (CR-1);

end

```

---

```
function varargout = GUI_(varargin)
```

(Not listed due to length ~ 2000 lines)

---

```

function [ HC_ratio ] = HCr( fueltype )
%   [ HC_ratio ] = HCr( fueltype )
%   HCR(fueltype) gives H to C ratio for a given fuel

switch(fueltype)
    case 'isoctane' % Heywood
        C=8; H=18;
    case 'diesel' % Heywood
        C=10.8; H=18.7;
    case 'gasoline' % Heywood
        C=8.26; H=15.5;
    case 'propane' % Heywood
        C=3; H=8;
end

HC_ratio = H / C;

```

---

```

function [ h ] = HFuel( fueltype )
%   [ h ] = HFuel( fueltype )
%
% HFuel returns the lower heating value as J/kg
switch fueltype
    case 'diesel'
        h = 44.0E6;
    case 'gasoline'
        h = 42.0E6;
    case 'isoctane'
        h = 44.3E6;
    case 'propane'
        h = 46.4E6;
end

end

```

---

```

function [ Cv M R ] = MProperties ( T, varargin )
% [ Cv M R ] = MProperties ( T, component, component ratio, ... )
% Example MProperties(350, 'O2', 1)
% gives the Cp and Molecular Mass of O2 at 350K
%
% Example MProperties(350, 'O2', 0.21, 'N2', 0.79)
% gives the Cp and Molecular Mass of air at 350K
%
% The ratios are normalised, i.e.:
% MProperties(350, 'O2', 0.21, 'N2', 0.79)
% is equal to:
% MProperties(350, 'O2', 1, 'N2', 3.7619)

numvarargs = size(varargin, 2);
if (mod(numvarargs, 2) == 1)
    error('Requires component and mole fraction for each component');
end

index_m = numvarargs/2;

tempCp = zeros(1, index_m);
tempM = zeros(1, index_m);
ratio = zeros(1, index_m);

index = 1;
for cnt = 1:2:numvarargs
    [tempCv(index) tempM(index)] = CProperties(T, varargin{cnt});
    ratio(index) = varargin{cnt+1};
    index = index +1;
end

norm = sum(ratio);
M = sum(tempM .* ratio)/norm;
Cv = sum(tempCv .* tempM .* ratio./norm) /M;
R = 8314.5 / M; %Eastop & McConkey kJ /kmolK

end



---


function [ dT ] = TCombustion( mode, mf, mc, xb1, xb2, h, Cv, varargin )
% [ dT ] = TCombustion( mode, mf, mc, xb1, xb2, h, Cv, [options] )
% dT = TCombustion( mode=1, mf, mc, xb_i, xb_i+1, h, Cv_u, Cv_b )
% or
% dT = TCombustion( mode=2, mf, mc, xb_i, xb_i+1, h, Cv )
%
% TCombustion estimates the temperature rise for a given change in
% fraction burn (xb_i to xb_i+1)
% Mode = 1: Frozen mixture composition for fresh air/air-fuel mix and
% exhaust gases, thus two specific heats (Cv_u, Cv_b).
% Mode = 2: The mixture properties are calculated external of this
% function and hence one specific heat is expected (Cv).
%
% Other Inputs:
% mf : total mass of fuel
% mc : mass of charge
% h : J/kg energy content of fuel
%
% Outputs:
% dT: Temperature rise

```

```

Ef = mf * h; % Calculate energy of the mass of fuel
if (xb2 < xb1) % Check xb is increasing
    disp('xb_i+1 < xb_i, is this expected?');
end

if mode == 1;
    numvarargs = size(varargin, 2);
    if (numvarargs ~=1 )
        error('Requires Cv for the burned mixture');
    end
    Cv_b = varargin{1};
    Cv_u = Cv;
    dT = (Ef*(xb2-xb1))/(mc*((1-xb2)*Cv_u+xb2*Cv_b));
else
    dT = (Ef*(xb2-xb1))/(mc*Cv);
end
end

```

---

```

function [ T2 ] = TCompression( mode, T1, P1, V1, V2, mc, Cv, varargin )
% [ T_i+1 ] = TCompression( mode=1, T_i, P_i, V_i, V_i+1, mc, Cv,
% [optional parameters] )
% [ T_i+1 ] = TCompression( mode=1, T_i, P_i, V_i, V_i+1, mc, Cv_u, Cv_b,
% xb)
% or
% [ T_i+1 ] = TCompression( mode=2, T_i, P_i, V_i, V_i+1, mc, Cv)
%
% TCompression estimates the temperature after a given change in volume.
% Mode = 1: Frozen mixture composition for fresh air/air-fuel mix and
% exhaust gases, thus two specific heats (Cv_u, Cv_b) are required as
% well as a fraction burn (xb).
% Mode = 2: The mixture properties are calculated external of this
% function and hence one specific heat is expected (Cv) and no fraction
% burn is expected.
%
% Other Inputs:
% T_i: Temperature at step i
% P_i: Pressure at step i
% V_i: Volume at step i
% V_i+1: Volume at step i+1
% mc: Mass of charge
%
% Outputs:
% T_i+1: Temperature at step i+1

if mode == 1;
    numvarargs = size(varargin, 2);
    if (numvarargs ~= 2 )
        error('Requires Cv for the burned mixture');
    end
    Cv_b = varargin{1};
    xb = varargin{2};
    Cv_u = Cv;
    T2 = T1 - P1*(V2-V1)/(mc*((1-xb)*Cv_u+xb*Cv_b));
else
    T2 = T1 - P1*(V2-V1)/(mc*Cv);
end
end

```

---

```

function [ B ] = UComposition( EquivilanceRatio, NOr, HCr, T, Mf, xb )
%   [ Unburned Mole Fraction Array ] = UComposition( EquivilanceRatio, NOr,
HCr, T, Mf, xb )
%   Where [...] = [ nFuel nO2 nN2 nCO2 nH2O nCO nH2 ]

eta = 4 / (4 + HCr);
if EquivilanceRatio <= 1
    nFuel = 4*(1-xb)*(1 + 2*eta)*EquivilanceRatio / Mf;
    nO2 = 1-xb*EquivilanceRatio;
    nN2 = NOr;
    nCO2 = xb*eta*EquivilanceRatio;
    nH2O = 2*xb*(1 - eta) * EquivilanceRatio;
    nCO = 0;
    nH2 = 0;
else
    K = exp(2.743 - 1.761E3/T - 1.611E6/T^2 + 0.2803E9/T^3);
    a = (K-1);
    b = -(K*(2*(EquivilanceRatio - 1) + eta*EquivilanceRatio) + 2*(1-
eta*EquivilanceRatio));
    c = 2*K*eta*EquivilanceRatio*(EquivilanceRatio-1);
    z = (-b-sqrt(b^2-4*a*c))/(2*a);
    nFuel = 4*(1-xb)*(1 + 2*eta)*EquivilanceRatio / Mf;
    nO2 = 1-xb;
    nN2 = NOr;
    nCO2 = xb*(eta*EquivilanceRatio - z);
    nH2O = xb*(2*(1 - eta*EquivilanceRatio) + z);
    nCO = xb*z;
    nH2 = xb*(2*(EquivilanceRatio - 1) - z);
end
B = [nFuel nO2 nN2 nCO2 nH2O nCO nH2];
n = sum(B);
B = B ./ n;
end

```

---

```

function [ Work ] = WDone( P, V )
%   [ Work ] = WDone( P, V )
%   WDone estimates the work done for a given set of P, V, values
temp = size(P,2);
Work = 0;

for cnt=2:temp
    Work = Work + (P(cnt)+P(cnt-1))/2*(V(cnt)-V(cnt-1));
end

```